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Differential Transform Method for the Kinetic Analysis of Thermal Inactivation of Enzyme as Applied in Biotechnology

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ABSTRACT

In this work, approximate analytical solution is developed using differential transformation method for finding the molar concentration of the native and denatured enzyme in terms of second-order rate constant. Also, the obtained solutions are used to study the kinetics of thermal inactivation of enzyme as applied in biotechnology. The analytical solution was validated with numerical solution using fourth- order Runge-Kutta. Good agreement was established between the numerical and approximated analytical solutions.

***Keywords*:** Kinetic analysis, Thermal inactivation, Enzyme, Analytical solution, Differential transformation method

1. INTRODUCTION

The importance and applications of urease as a good catalyst for hydrolysis of urea has attracted several research interests especially in biotechnology and biomedical engineering studies [1-12]. The study of kinetic inactivation of the enzyme requires the development of

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mathematical models and provision of analytical solutions that will provide physical insights into the phenomena. Although, three step mechanism of thermal inactivation reaction model has been developed there is no provision of analytical solutions (except Ananthi *et al*. [13]) for the predictions of model concentrations of the native enzyme, denature enzyme and temperature for thermal inactivation of urease. Ananthi *et al*. [13] applied homotopy perturbation techniques for the analysis of kinetivc and thermal inactivation of the enzyme. However, the use of HAM in the analysis of linear and nonlinear equations requires the determination of auxiliary parameter which will increase the computational cost and time. Moreover, such method requires high skill in mathematical analysis. Consequently, a direct and relatively simple method is needed to establish analytical solution for the kinetic of thermal inactivation of urease. Therefore, in this work, differential transformation method (DTM) is used to analyse the problem.

Differential transform method is an analytical method for solving differential equations most of the analytical (exact or approximation) and purely numerical methods are computationally intensive or required symbolic computation for the calculation of higher order derivatives as in Taylor's method. Although, this concept was introduced by Zhou (1986), its applications to both linear and non-linear differential and system of differential equation have fast gained ground or appeared in many engineering and scientific research. It is a semi-anlytical/semi-numerical technique that depends on Taylor's Series (Arikoglu and Ozkol (2008) which could solve differential equations, difference equation, differential-difference equations, fractional differential equation, pantograph equation and integro-differential equation. The method is applied to solve many non-linear integral and differential equations without linearization, discretization or perturbation i.e. it shows it advantages over pure numerical schemes since no discretization is needed and over the known analytical method for solving non-linear differential equation since it requires no approximation, linearization or perturbation. DTM reduces the computational difficulties of the other traditional methods and also the calculations can be made with simple manipulations (Odibat, 2008).

The classical or traditional Taylor series method requires a lot of symbolic for the derivatives of functions, it takes a lot of computational time for higher order derivatives. Hence, it could be referred to as an updated version of the Taylor series method. The method determines the coefficient of the Taylor series of the function by solving the induced recursive equation from the given equation. Using DTM, a closed form series solution or approximate solution can be obtained. It provides excellent approximations to the solution of non-linear equation with high accuracy. It provides more accurate solution or result than Variation Iteration Method (VIM) (Salehi (2012)).

DTM constructs an analytic solution in the form of a finite difference and Rk4 polynomial which is widely equivalent explicit form of solution. It solves problems (non-linear) without linearization, restrictive assumptions perturbation and discretization round-off errors complexity of expansion of derivatives and compute derivatives symbolically. DTM is a numerical as well as analytical method in nature (semi-numerical analytical method). It is an iterative procedure for obtaining analytical Taylor series solution of differential equations.

It is capable of greatly reducing the size of computational work while still accurately providing the series solution with fast convergence rate. Unlike most numerical techniques, it provides a closed-form solution. Also, DTM can be used to solve linear and non-linear non-homogeneous PDEs with accurate approximate, which is acceptable for small range, because of boundary conditions are satisfied via the method (DTM), and the remaining unsatisfied conditions play no roles in the final results (Madani *et al.* 2011).

Laplace transform could be combined with the DTM to overcome this deficiency that is mainly caused by the unsatisfied conditions. DTM is more effective and convenient compared to the ADM and VIM. DTM does not require many computations as carried out in ADM and VIM to have high and fast rate of convergence. An analytical expression is more convenient for engineering calculations compare with experimental or numerical studies and is also obvious starting point for a better understanding of the relationship between the physical quantities/propancy. The semi-analytical solution/method would provide continuous physical insights than pure numerical computation/method. Therefore, in this work, approximate analytical solutions are developed using differential transformation for finding the molar concentration of the native and denatured enzyme in terms of second-order rate constant. Also, the obtained solutions are used to study the kinetics of thermal inactivation of enzyme as applied in biotechnology. The analytical solutions were validated with numerical solutions (Runge - Kutta) and good agreements were established.

2. MODEL FORMULATION

The three – step mechanism of inactivation with a dissociation reaction of the native form of the enzyme, N, into a denatured form, D, and with two parallel association reactions of the native and denatured forms into irreversible denatured enzymes forms I_1 and I_2, respectively:

$$N \underset{k_{-1}}{\overset{k_{+1}}{\Leftrightarrow}} 2D \qquad 2D \overset{k_2}{\rightarrow} I_1 \qquad 2N \overset{k_3}{\rightarrow} I_2 \tag{1}$$

where: k_{+1}, k_{-1}, k_2 and k_3 represent the rate constants of individual reactions. The material balances equations for N, D and temperatures are given as follows [1]:

$$\frac{dC_N}{dt} = -k_{+1}C_N + k_{-1}{C_D}^2 - 2k_3{C_N}^2 \tag{2a}$$

$$\frac{dC_D}{dt} = 2k_{+1}C_N - 2(k_{-1} + k_2){C_D}^2 \tag{2b}$$

$$\frac{dT}{dt} = K(T_B - T) \tag{2c}$$

Initial conditions

$$t = 0,\ C_N = 1, \quad C_D = 0 \qquad T = 30 + T_B \tag{3}$$

3. BASIC DEFINITIONS OF DIFFERENTIAL TRANSFORM METHOD

If $u(t)$ is analytic in the domain T, then it will be differentiated continuously with respect to time t.

$$\frac{d^K u(t)}{dt^K} = \phi(t,k) \qquad \text{for} \qquad \text{all } t \in T \tag{4}$$

for $t = t_i$, then $\phi(t,k) = \phi(t_i, K)$, where K belongs to the set of non-negative integers, denoted as the K-domain. Therefore eq. (1) can be rewritten as

$$U(k) = \phi(t_i, k) = \left[\frac{d^k u(t)}{dt^K}\right]_{t=t_i} \tag{5}$$

where: U_k is called the spectrum of $u(t)$ at $t = t_i$

If $u(t)$ can be expressed by Taylor's series, the $u(t)$ can be represented as:

$$u(t) = \sum_k^{\infty} \left[\frac{(t-t_i)^K}{k!}\right] U(k) \tag{6}$$

where: Equ. (7) is called the inverse of $U(k)$ using the symbol 'D' denoting the differential transformation process and combining (6) and (7), it is obtained that

$$u(t) = \sum_{K=0}^{\infty} \left[\frac{(t-t_i)^K}{K!}\right] U(k) = D^{-1} U(k) \tag{7}$$

3. 1. Operational Properties of Differential Transformation Method

If $u(t)$ *and* $v(t)$ are two independent functions with time (t) where $U(k)$ and $V(k)$ are the transformed function corresponding to $u(t)$ and $v(t)$, then it can be proved from the fundamental mathematics operations performed by differential transformation that.

(1) If $z(t) = u(t) \pm v(t)$, then $Z(k) = U(k) \pm V(k)$

(2) If $z(t) = \alpha u(t)$, then $Z(k) = \alpha U(k)$

(3) If $z(t) = \dfrac{du(t)}{dt}$, then $Z(k) = (k-1)\, U(k+1)$

(4) If $z(t) = u(t)v(t)$, then $Z(t) = \sum_{i=0}^{k} V(l) U(k-l)$

(5) If $z(t) = u^m(t)$, then $Z(t) = \sum_{I=0}^{k} U^{m-1}(l) U(k-l)$

(6) If $z(t) = u^n(t) v^n(t)$, then $Z(t) = \sum_{l-0}^{k} \left[\sum_{j=0}^{l} [V(j)U(l-j)] \sum_{j=0}^{k-l} [V(j)U(k-l-j)] \right]$

(7) If $z(t) = u(t)v(t)$, then $Z(k) = \sum_{l=0}^{k} (l+1)V(l+1)U(k-l)$

3. 2. Analysis of the Kinetic Models using Differential Transformation Method

For the sake of conveniences in the analysis, let $C_N = x$, $C_D = y$, $k_{+1} = a$, $k_{-1} = b$, $k_2 = c$ and $k_3 = d$. Therefore, Eq. (2a-2c) becomes

$$\frac{dx}{dt} = -ax + by^2 - 2dx^2 \quad (8a)$$

$$\frac{dy}{dt} = 2ax - 2(b+c)y^2 \quad (8b)$$

$$t = 0, \quad x = 1, \quad y = 0 \quad (8c)$$

The recursive expression by differential transformation method is given as

$$(p+1)\, X[p+1] = -a\, X[p] + b \sum_{i=0}^{P} Y[i]\, Y[p-i] - 2d \sum_{i=0}^{P} X[i]\, X[[p-i] \quad (9a)$$

$$(p+1)\, Y[p+1] = 2a\, X[p] - 2(b+c) \sum_{i=0}^{P} Y[i]\, Y[p-i] \quad (9b)$$

$$\text{Initial Conditions} \quad X(0) = 1, \quad Y(0) = 1 \quad (9c)$$

At $p = 0$

$X[0] = 1$

$Y[0] = 0$

At $p = 1$

$X[1] = -a - 2d$

$Y[1] = 2a$

At $p = 2$

$X[2] = \frac{1}{2}(a + 2d)(a + 4d)$

$Y[2] = -a(a + 2d)$

At $p = 3$

$X[3] = \frac{1}{6}(-a^3 + 8a^2b - 14a^2d - 48ad^2 - 48d^3)$

$Y[3] = \frac{1}{3}a(a^2 - 8ab - 8ac + 6ad + 8d^2)$

At $p=4$

$$X[4]=\frac{1}{24}(a^4-32a^3b+30a^3d-80a^2bd+200a^2d^2+480ad^3+384d^4)$$

$$Y[4]=-\frac{1}{12}a(a^3-32a^2b-24a^2c+14a^2d-48abd-48acd+48ad^2+48d^3)$$

At $p=5$

$$X[5]=\frac{1}{120}(-a^5+88a^4b-256a^3b^2-256a^3bc-62a^4d+624a^3bd-720a^3d^2+928a^2bd^2-3120a^2d^3-5760ad^4-3840d^5)$$

$$Y[5]=\frac{1}{60}a(a^4-88a^3b+256a^2b^2-56a^3c+512a^2bc+256a^2c^2+30a^3d-368a^2bd-288a^2cd+200a^2d^2-352abd^2-352acd^2+480ad^3+384d^4)$$

At $p=6$

$$X[6]=\frac{1}{720}(a^6-208a^5b+2176a^4b^2+1856a^4bc+126a^5d-3136a^4bd+4224a^3b^2d+4224a^3bcd+2408a^4d^2-11744a^3bd^2+16800a^3d^3-12672a^2bd^3+53760a^2d^4+80640ad^5+46080d^6)$$

$$Y[6]=-\frac{1}{360}a(a^5-208a^4b+2176a^3b^2-120a^4c+3776a^3bc+1600a^3c^2+62a^4d-1824a^3bd+3200a^2b^2d-1200a^3cd+6400a^2bcd+3200a^2c^2d+720a^3d^2-4448a^2bd^2-3520a^2cd^2+3120a^2d^3-3200abd^3-3200acd^3+5760ad^4+3840d^5)$$

At $p=7$

$$X[7]=\frac{1}{5040}(-a^7+456a^6b-11520a^5b^2+17408a^4b^3-8704a^5bc+34816a^4b^2c+17408a^4bc^2-254a^6d+12960a^5bd-60416a^4b^2d-50816a^4bcd-7728a^5d^2+91648a^4bd^2-67840a^3b^2d^2-67840a^3bcd^2-81648a^4d^3+234752a^3bd^3-403200a^3d^4+199424a^2bd^4-1021440a^2d^5-1290240ad^6-645120d^7)$$

$$Y[7]=\frac{1}{2520}a(a^6-456a^5b+11520a^4b^2-17408a^3b^3-248a^5c+18048a^4bc-52224a^3b^2c+6848a^4c^2-52224a^3bc^2-17408a^3c^3+126a^5d-7456a^4bd+43008a^3b^2d-4320a^4cd+76032a^3bcd+33024a^3c^2d+2408a^4d^2-34624a^3bd^2+38656a^2b^2d^2-22880a^3cd^2+77312a^2bcd^2+38656a^2c^2d^2+16800a^3d^3-60672a^2bd^3-48000a^2cd^3+53760a^2d^4-35072abd^4-35072acd^4+80640ad^5+46080d^6)$$

At $p=8$

$$X[8]=\frac{1}{40320}(a^8-960a^7b+49152a^6b^2-253952a^5b^3+33792a^6bc-457728a^5b^2c\\ -203776a^5bc^2+510a^7d-48048a^6bd+516864a^5b^2d\\ -442368a^4b^3d+378624a^5bcd-884736a^4b^2cd-442368a^4bc^2d\\ +24200a^6d^2-570432a^5bd^2+1459968a^4b^2d^2+1217280a^4bcd^2\\ +372960a^5d^3-2601216a^4bd^3+1192448a^3b^2d^3+1192448a^3bcd^3\\ +2669184a^4d^4-5064704a^3bd^4+10160640a^3d^5-3550208a^2bd^5\\ +21288960a^2d^6+23224320ad^7+10321920d^8)$$

$$Y[8]=-\frac{1}{20160}a(a^7-960a^6b+49152a^5b^2-253952a^4b^3-504a^6c+71424a^5bc\\ -694272a^4b^2c+25088a^5c^2-626688a^4bc^2-186368a^4c^3+254a^6d\\ -27408a^5bd+352512a^4b^2d-372736a^3b^3d-14448a^5cd\\ +562432a^4bcd-1118208a^3b^2cd+219520a^4c^2d-1118208a^3bc^2d\\ -372736a^3c^3d+7728a^5d^2-214848a^4bd^2+759552a^3b^2d^2\\ -123200a^4cd^2+1354496a^3bcd^2+594944a^3c^2d^2+81648a^4d^3\\ -682752a^3bd^3+512512a^2b^2d^3-448000a^3cd^3+1025024a^2bcd^3\\ +512512a^2c^2d^3+403200a^3d^4-935936a^2bd^4-736512a^2cd^4\\ +1021440a^2d^5-451584abd^5-451584acd^5+1290240ad^6\\ +645120d^7)$$

At $p=9$

$$X[9]=\frac{1}{362880}(-a^9+1976a^8b-185856a^7b^2+2195456a^6b^3-2031616a^5b^4\\ -118656a^7bc+3634176a^6b^2c-6094848a^5b^3c+1477120a^6bc^2\\ -6094848a^5b^2c^2-2031616a^5bc^3-1022a^8d+166608a^7bd\\ -3449856a^6b^2d+9785344a^5b^3d-2258688a^6bcd+17512448a^5b^2cd\\ +7727104a^5bc^2d-74640a^7d^2+3114336a^6bd^2-18216192a^5b^2d^2\\ +9615360a^4b^3d^2-13099264a^5bcd^2+19230720a^4b^2cd^2\\ +9615360a^4bc^2d^2-1637040a^6d^3+22479360a^5bd^3\\ -35897856a^4b^2d^3-29738496a^4bcd^3-16329600a^5d^4\\ +75234816a^4bd^4-23255040a^3b^2d^4-23255040a^3bcd^4\\ -87655680a^4d^5+118098944a^3bd^5-270950400a^3d^6\\ +70469632a^2bd^6-483840000a^2d^7-464486400ad^8-185794560d^9)$$

$$Y[9] = \frac{1}{181440} a(a^8 - 1976a^7b + 185856a^6b^2 - 2195456a^5b^3 + 2031616a^4b^4 - 1016a^7c + 255360a^6bc - 5575680a^5b^2c + 8126464a^4b^3c + 84864a^6c^2 - 4653568a^5bc^2 + 12189696a^4b^2c^2 - 1273344a^5c^3 + 8126464a^4bc^3 + 2031616a^4c^4 + 510a^7d - 94416a^6bd + 2282496a^5b^2d - 7753728a^4b^3d - 46368a^6cd + 3345408a^5bcd - 21420032a^4b^2cd + 1201152a^5c^2d - 19578880a^4bc^2d - 5912576a^4c^3d + 24200a^6d^2 - 1169184a^5bd^2 + 8904960a^4b^2d^2 - 6731776a^3b^3d^2 - 598752a^5cd^2 + 14323456a^4bcd^2 - 20195328a^3b^2cd^2 + 5661184a^4c^2d^2 - 20195328a^3bc^2d^2 - 6731776a^3c^3d^2 + 372960a^5d^3 - 5961216a^4bd^3 + 13920768a^3b^2d^3 - 3360000a^4cd^3 + 24920576a^3bcd^3 + 10999808a^3c^2d^3 + 2669184a^4d^4 - 14393856a^3bd^4 + 7606272a^2b^2d^4 - 9329152a^3cd^4 + 15212544a^2bcd^4 + 7606272a^2c^2d^4 + 10160640a^3d^5 - 16194560a^2bd^5 - 12644352a^2cd^5 + 21288960a^2d^6 - 6690816abd^6 - 6690816acd^6 + 23224320ad^7 + 10321920d^8)$$

At $p = 10$

$$X[10] = \frac{1}{3628800}(a^{10} - 4016a^9b + 652416a^8b^2 - 14729216a^7b^3 + 45285376a^6b^4 + 393024a^8bc - 22726656a^7b^2c + 125829120a^6b^3c - 8588800a^7bc^2 + 115802112a^6b^2c^2 + 35258368a^6bc^3 + 2046a^9d - 552992a^8bd + 19870080a^7b^2d - 125067264a^6b^3d + 74579968a^5b^4d + 11861376a^7bcd - 203614208a^6b^2cd + 223739904a^5b^3cd - 81081344a^6bc^2d + 223739904a^5b^2c^2d + 74579968a^5bc^3d + 228008a^8d^2 - 15631008a^7bd^2 + 173158656a^6b^2d^2 - 300335104a^5b^3d^2 + 110142208a^6bcd^2 - 534751232a^5b^2cd^2 - 234416128a^5bc^2d^2 + 6996000a^7d^3 - 167505024a^6bd^3 + 611667456a^5b^2d^3 - 213356544a^4b^3d^3 + 434254336a^5bcd^3 - 426713088a^4b^2cd^3 - 213356544a^4bc^2d^3 + 94744320a^6d^4 - 856747008a^5bd^4 + 930398208a^4b^2d^4 + 766973952a^4bcd^4 + 689230080a^5d^5 - 2258736128a^4bd^5 + 500871168a^3b^2d^5 + 500871168a^3bcd^5 + 2948520960a^4d^6 - 2968922112a^3bd^6 + 7664025600a^3d^7 - 1542111232a^2bd^7 + 11921817600a^2d^8 + 10218700800ad^9 + 3715891200d^{10})$$

$$
\begin{aligned}
Y[10] = -\frac{1}{1814400}a(&a^9 - 4016a^8b + 652416a^7b^2 - 14729216a^6b^3 + 45285376a^5b^4 \\
&- 2040a^8c + 859584a^7bc - 35260416a^6b^2c + 169082880a^5b^3c \\
&+ 274368a^7c^2 - 27681280a^6bc^2 + 235536384a^5b^2c^2 - 7111680a^6c^3 \\
&+ 144965632a^5bc^3 + 33226752a^5c^4 + 1022a^8d - 311808a^7bd \\
&+ 12859776a^6b^2d - 94658560a^5b^3d + 66453504a^4b^4d - 145200a^7cd \\
&+ 17574144a^6bcd - 243341312a^5b^2cd + 265814016a^4b^3cd \\
&+ 5905536a^6c^2d - 206285824a^5bc^2d + 398721024a^4b^2c^2d \\
&- 57603072a^5c^3d + 265814016a^4bc^3d + 66453504a^4c^4d + 74640a^7d^2 \\
&- 5849376a^6bd^2 + 80992512a^5b^2d^2 - 190267392a^4b^3d^2 \\
&- 2735040a^6cd^2 + 118961920a^5bcd^2 - 528789504a^4b^2cd^2 \\
&+ 43086336a^5c^2d^2 - 486776832a^4bc^2d^2 - 148254720a^4c^3d^2 \\
&+ 1637040a^6d^3 - 44722560a^5bd^3 + 221326848a^4b^2d^3 \\
&- 122990592a^3b^3d^3 - 22243200a^5cd^3 + 356894208a^4bcd^3 \\
&- 368971776a^3b^2cd^3 + 141726720a^4c^2d^3 - 368971776a^3bc^2d^3 \\
&- 122990592a^3c^3d^3 + 16329600a^5d^4 - 168035328a^4bd^4 \\
&+ 273917952a^3b^2d^4 - 92800512a^4cd^4 + 490967040a^3bcd^4 \\
&+ 217049088a^3c^2d^4 + 87655680a^4d^5 - 326730752a^3bd^5 \\
&+ 126173184a^2b^2d^5 - 208631808a^3cd^5 + 252346368a^2bcd^5 \\
&+ 126173184a^2c^2d^5 + 270950400a^3d^6 - 311339008a^2bd^6 \\
&- 240869376a^2cd^6 + 483840000a^2d^7 - 112214016abd^7 \\
&- 112214016acd^7 + 464486400ad^8 + 1857945
\end{aligned}
$$

Hence, the solution is

$$
\begin{aligned}
X(t) = {} & X[0] + X[1]t + X[2]t^2 + X[3]t^3 + X[4]t^4 + X[5]t^5 + X[6]t^6 \\
& +X[7]t^7 + X[8]t^8 + X[7]t^7 + X[8]t^8 + X[9]t^9 + X[10]t^{10}
\end{aligned} \tag{10}
$$

$$
\begin{aligned}
Y(t) = {} & Y[0] + Y[1]t + Y[2]t^2 + Y[3]t^3 + Y[4]t^4 + Y[5]t^5 + Y[6]t^6 \\
& +Y[7]t^7 + Y[8]t^8 + Y[7]t^7 + Y[8]t^8 + Y[9]t^9 + Y[10]t^{10}
\end{aligned} \tag{11}
$$

4. RESULTS AND DISCUSSION

Equations (10) and (11) represent the analytical expression of concentrations of native and denatured enzyme for all values of parameters. These analytical solutions are verified with the numerical solutions

Tables 1 and 2 show the comparison between the results of differential transformation method (DTM) and numerical method (NM) using Fourth-order Runge-Kutta method coupled with shooting method. The obtained results of velocity distributions using DTM as compared with the numerical procedure are in good agreements.

The high accuracy of DTM gives high confidence about validity of the method in providing solutions to the problem. It should be noted that a, b, c and d represent the rate constants of individual reactions which are k_{+1}, k_{-1}, k_2 and k_3, respectively.

Table 1. Comparison of results (X(t)).

The results of DTM and Numerical methods for X(t) for $a = 1, \; b = 0.01, \; c = 0.001, \quad d = 0.05$
X(t)

X	**DTM**	**NUM**	**Residue of DTM**
0.00	1.000000	1.000000	0.000000
0.10	0.896320	0.896320	0.000000
0.20	0.804239	0.804239	0.000000
0.30	0.722362	0.722362	0.000000
0.40	0.649479	0.649479	0.000000
0.50	0.584542	0.584542	0.000000
0.60	0.526638	0.526637	0.000001
0.70	0.474968	0.474965	0.000003
0.80	0.428836	0.428824	0.000012
0.90	0.387641	0.387599	0.000042
1.00	0.350878	0.350748	0.000130

Table 2. Comparison of results (Y(t)).

The results of DTM and Numerical methods for X(t) for $a = 1, \; b = 0.01, \; c = 0.001, \quad d = 0.05$
Y(t)

X	**DTM**	**NUM**	**Residue of DTM**
0.00	0.000000	0.000000	0.000000
0.10	0.189399	0.189399	0.000000
0.20	0.359101	0.359101	0.000000
0.30	0.511178	0.511178	0.000000
0.40	0.647477	0.647477	0.000000
0.50	0.769644	0.769644	0.000000
0.60	0.879150	0.879150	0.000000
0.70	0.977312	0.977311	0.000001
0.80	1.065300	1.065300	0.000000
0.90	1.144180	1.144170	0.000010
1.00	1.214880	1.214840	0.000040

The developed solutions in Eqs. (10) and (11) are simulated in MATHEMATICA and the results are presented in Figs. 1-6.

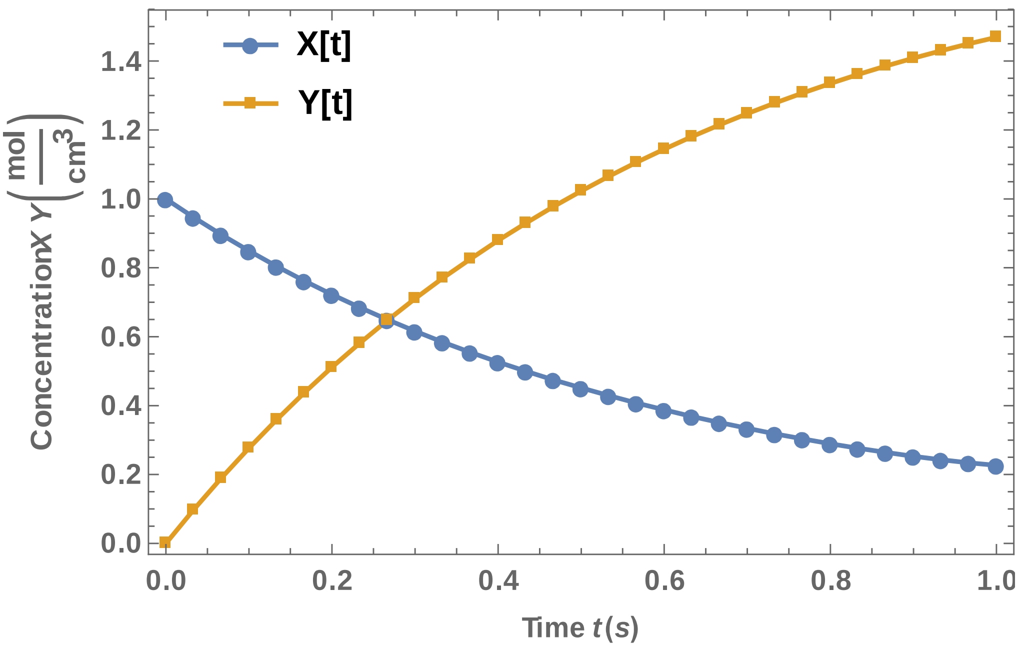

Figure 1. Molar concentration of N and D versus time t for
$a = 1, \; b = 0.01, \quad c = 0.001, \quad d = 0.05$

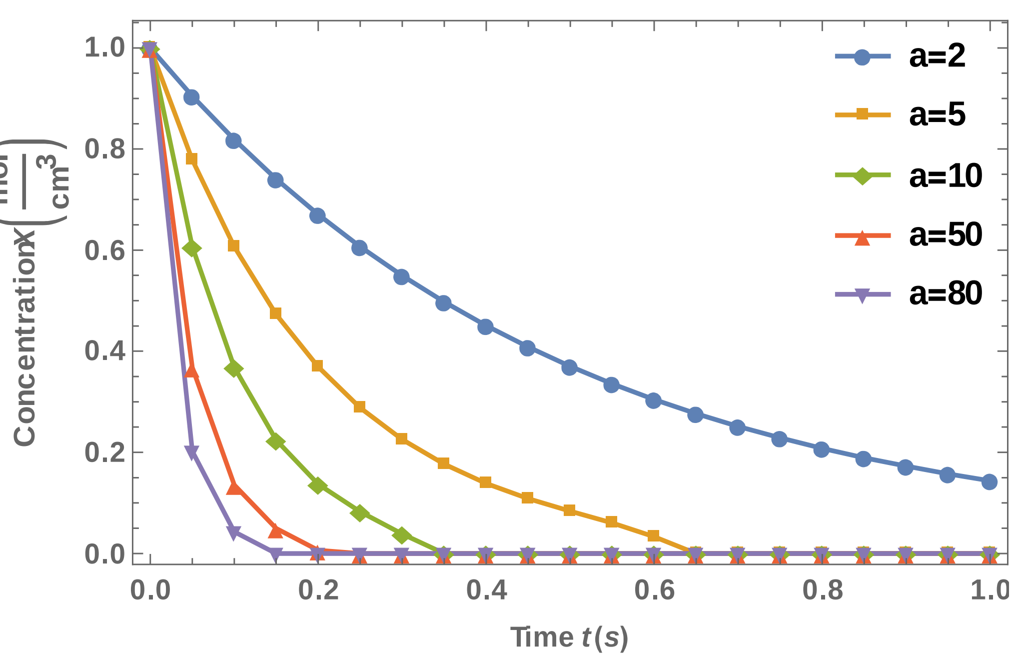

Figure 2. Molar concentrations of N and D versus time t for
$x[t]; \quad b = 0.01, c = 0.001, d = 0.001$

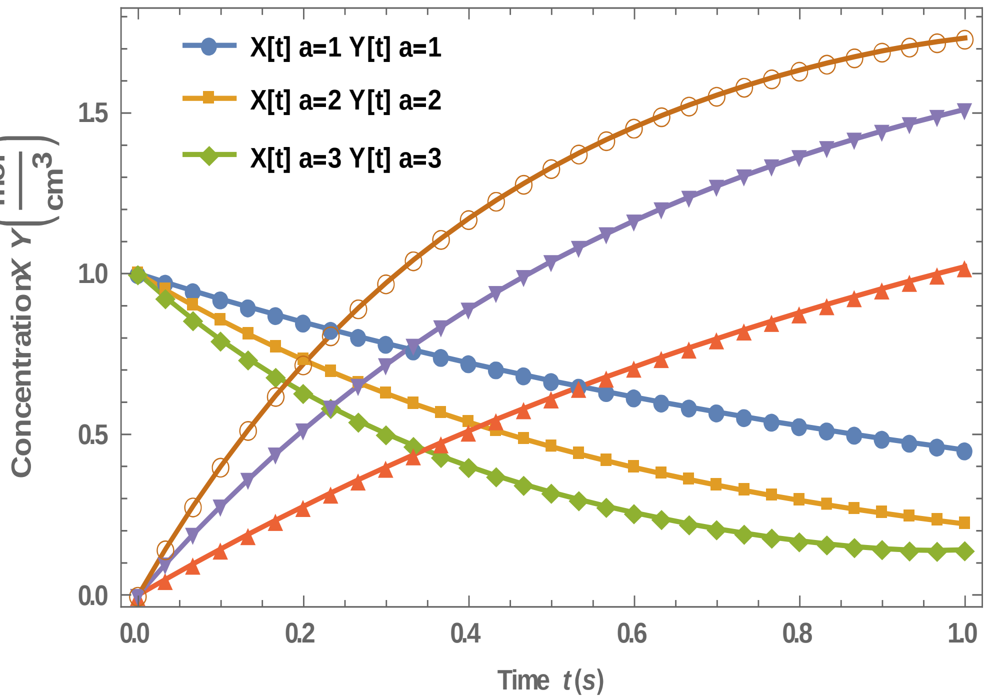

Figure 3. Molar concentrations of N and D versus time t for
$Y[t]$; $b = 0.01, c = 0.001, d = 0.001$

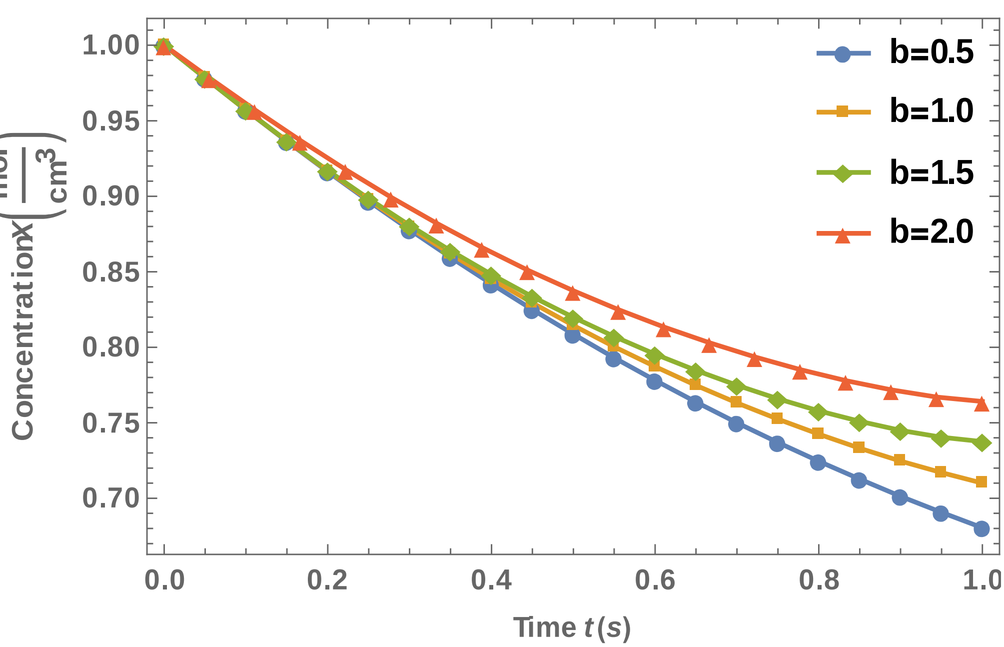

Figure 4. Molar concentrations of N and D versus time t for
$X[t]$; $a = 0.88$, $c = 0.001$, $d = 0.00028$

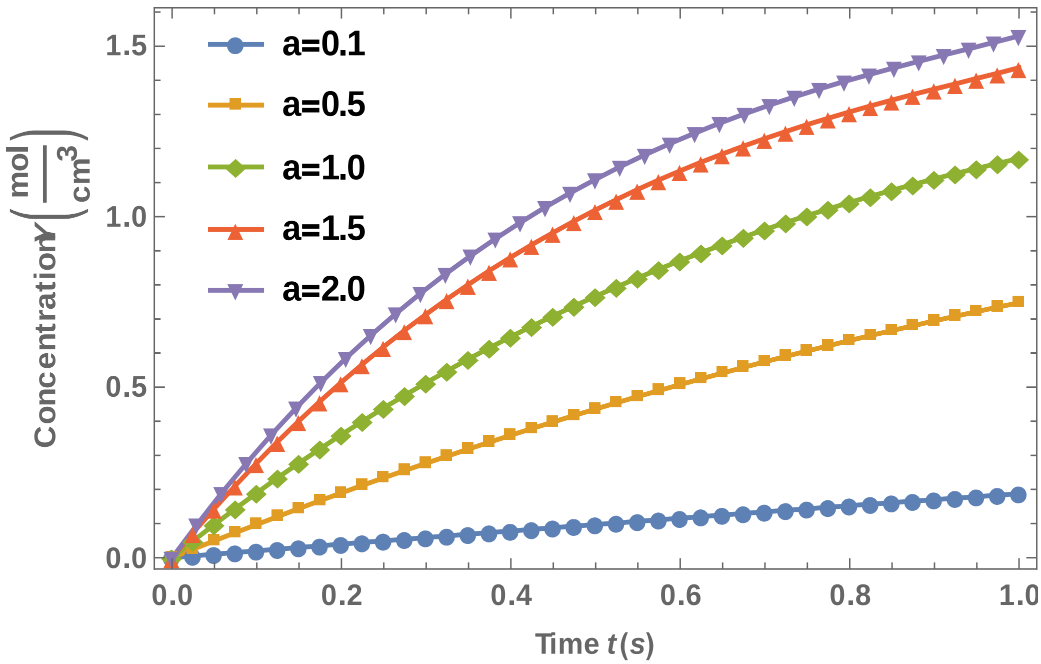

Figure 5. Molar concentrations of N and D versus time t for $Y[t]; \ \ b = 0.1, \quad c = 0.000266, \ \ d = 0.001$

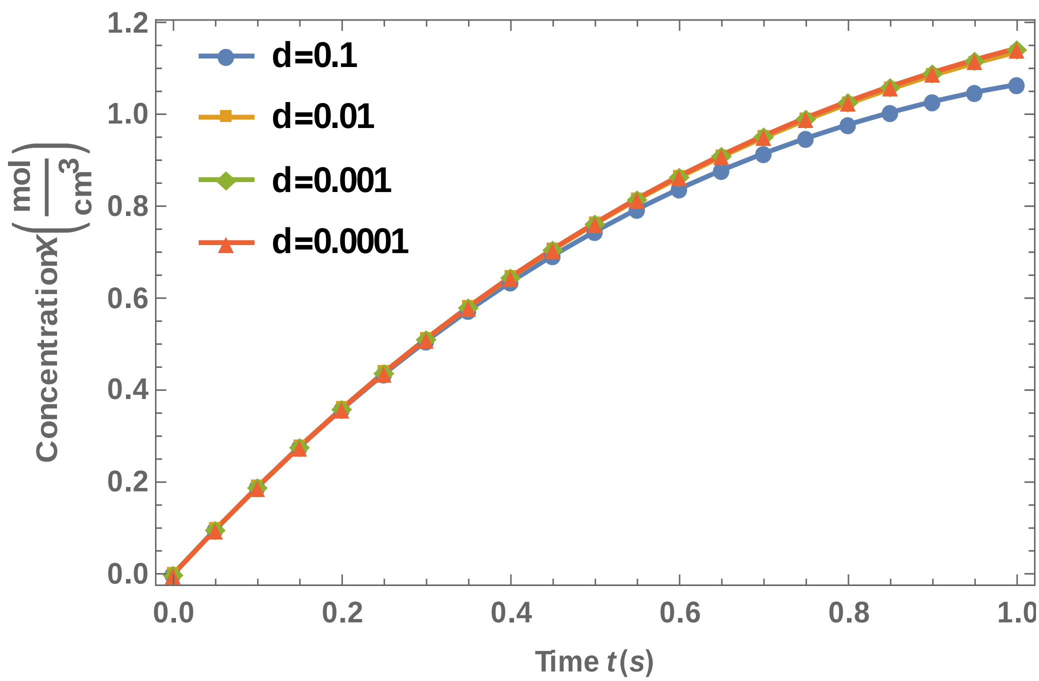

Figure 6. Molar concentrations of N and D versus time t for $Y[t]; \ \ a = 1, \quad c = 0.1, \ \ d = 0.001$

Figures 1-6 represent the molar concentrations for various values of rate constant. From the figure, it is inferred that, when time increases the concentration of c_N decreases whereas the concentration of c_D increases. The time taken to reach the maximum value of c_D is the same as the time taken to reach the minimum value of c_N. The steady value of c_D and c_N depends upon the rate constants. Figures 2(a)–2(c) represent the molar concentration of C_N versus time t for various values of rate constant k_{+1} and k_{-1}. From that figure, it is observed that, c_N increases when k_{+1} and k_{-1} increase. Figure 3 represents the molar concentration of c_D versus time t for various values of parameter k_{+1}. From this figure, it is found that, the value of concentration c_D initially increases and reaches the steady state value when $t \geq 5$. The concentration c_D increases when k_{+1} increases. The concentration becomes zero when $k_{+1} \leq 0.01$ s^{-1}. Figure 1(e) denotes the representation temperature T versus time t for various values of T_B.The value of temperature increases when T_B increases. It is almost linear with respect to time t.

6. CONCLUSIONS

In this work, we obtained the analytical expression of concentrations in terms of rate constants k bath temperature T_B, and coefficient in the enthalpy balance K. The nonlinear ordinary differential equations have been solved analytically. The closed analytical expressions of molar concentrations of c_N, c_D, and temperature T are obtained using the differential transformation method. An agreement with the numerical result is noted. The information gained from this theoretical model can be useful for the kinetic analysis of the experimental results over handling rate constants and molar concentrations.

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