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The New Homotopy Perturbation Method (NHPM) for Nonlinear Parabolic Equation in Chemical Sciences

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Abstract: In this paper, we have presented new homotopy perturbation method (NHPM) to solve the system of nonlinear parabolic equation in chemical sciences. The NHPM allows for the solution of the nonlinear parabolic equations to be calculated in the form of a series with easily computable term by converting a non-linear differential equation into linear differential equation. The obtained results are presented and only one iteration is required to obtain an approximate solution that is accurate and efficient. Simple analytical expressions for the concentration of substrate and product have been derived for all values of reaction parameters using the new homotopy perturbation method (NHPM). The analytical results are also compared with numerical ones and a good agreement is obtained.

MSC: 34B15, 34B60.

Keywords: Nonlinear equation, New homotopy perturbation method, Parabolic equation.

1. Introduction

Many physical real life problems can be described by mathematical models that involves linear or nonlinear partial differential equations. Mathematical modeling involves physical observation, selection of the relevant physical variables, formulation of the mathematical equations, analysis of the equations, simulation, and finally, validation of the model with experimental/numerical. The behavior of each model is governed by the input data for the particular problem: the boundary and initial conditions, the coefficient functions of the differential equation, and the forcing function. This input data cause the solution of the model problem to possess highly localized properties in space, in time, or in both. Thus, the investigation of the exact or approximate solution helps us to understand the means of these mathematical models. In most case, it is complicated, to find the exact and analytical solution of the nonlinear problems and even if it is obtained, the steps used for calculation maybe too complicated. Numerical solutions or approximate analytical solutions become necessary for these problem. The main goal of this paper is to apply the new homotopy perturbation method (NHPM) to obtain the approximate solution of the system of nonlinear parabolic differential equations with nonlocal boundary conditions. Parabolic equations in one dimension that involve non local boundary conditions have been studied by several authors [1-5].

Approximate analytical schemes such as Adomain decomposition method (ADM), Variational iteration method (VIM), Homotopy perturbation method (HPM) and Homotopy analysis method (HAM) have been used to solve the any linear

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nonlinear problems. The solution obtained by using these methods shows the applicability, accuracy and efficiency in solving a large class of nonlinear physics, engineering and various branches of mathematics. The Homotopy perturbation method (HPM), was first proposed by He in 1998, was developed and improved by He [6-8]. The HPM is a novel and effective method, and can solve various nonlinear equations of various branches in mathematics and physical or chemical sciences. This method has been successfully applied to solve many types of problems [9-12].

The purpose of this communication is to derive the analytical expression of concentrations and current of four enzyme systems based on new homotopy perturbation method. This is an effective tool for solve the system of nonlinear problems in chemical sciences. These analytical results are helpful to understand the mechanism and physical effects of parameters through the mathematical modeled problems. It is also useful to validate the numerical results and the experimental data.

2. Mathematical Formulation of the Problem And Analysis

The reaction of the enzyme in cylindrical electrode are [13]:

$$\mathrm{O_2}+2\ \text{catechol} \rightarrow\ 2\ O-\text{quinone} + 2\ \mathrm{H_2O} \tag{1}$$

$$O-\text{quinone}\ + 2\,\mathrm{H^+} + 2\,\mathrm{e^-}\ \rightarrow\ \text{catechol} \tag{2}$$

The electrode conversion is made in presences of stirred solution containing an excess of supporting electrolyte, in three different states, oxy, met, deoxy [14]. Hence, the catechol/quinone conversion forms an amplification cycle within the enzyme film.

$$[\mathrm{Cu(I)-Cu(I)}]_{\mathrm{deoxy}} + \mathrm{O_2} + 2\mathrm{H_2O} \xrightarrow{k_1} [\mathrm{H_2O-Cu(II)-O-O-Cu(II)-H_2O}]_{\mathrm{oxy}} \tag{3}$$

$$[\mathrm{H_2O-Cu(II)-O-O-Cu(II)-H_2O}]_{\mathrm{oxy}} \xrightarrow{k_2} [\mathrm{Cu(II)-Ca-Cu(II)}]_{\mathrm{met}} + 2\mathrm{H_2O} + 2\mathrm{H^+} \tag{4}$$

$$[\mathrm{Cu(II)-Ca-Cu(II)}]_{\mathrm{met}} \xrightarrow{k_3} [\mathrm{Cu(I)-Cu(I)}]_{\mathrm{deoxy}} + \mathrm{Q} \tag{5}$$

In these stages, the enzyme concentration is supposed as unbroken and that the enzyme reaction follows Michaelis-Menten kinetics, in the reaction in the film is [15]

$$S + E_1 \underset{k_2}{\overset{k_1}{\rightleftarrows}} [E_1S] \xrightarrow{k_{cat}} P + E_2 \tag{6}$$

where

$$k_{cat} = k_1 c_{O_2} \quad \text{and} \quad K_M = \frac{k_1(k_2+k_3)c_{O_2}}{k_2k_3} \tag{7}$$

are the rate constant and Michaelis-Menten constant. The mass balance for concentration of catechol c_C can be written as follows:

$$\frac{D_C}{r}\frac{d}{dr}\left(r\frac{dc_C}{dr}\right) - \frac{k_{cat}c_Ec_C}{c_C+K_M} = 0 \tag{8}$$

Where c_C, c_E and c_Q is the concentration profile of catechol, enzyme and quinone respectively D_C and $D_Q$are its diffusion coefficients, and K_M is the Michaelis constant. Then the equation of continuum for quinone is generally expressed in the steady-state by [13]

$$\frac{D_Q}{r}\frac{d}{dr}\left(r\frac{dc_Q}{dr}\right) + \frac{k_{cat}c_Ec_C}{c_C+K_M} = 0 \tag{9}$$

At the electrode surface (r_0) and at the film surface (r_1) the boundary conditions are given by [13]

$$\begin{aligned} r = r_0: &\quad c_C = c_C^*, \quad c_Q = 0 \\ r = r_1: &\quad c_C = c_C^*, \quad c_Q = 0 \end{aligned} \tag{10}$$

where c_C^* is the bulk concentration of catechol scaled by the partition coefficient of the enzyme film. Relation between the concentrations catechol and quinone is obtained by adding the equations (8) and (9) and integrating with boundary condition (10):

$$\frac{c_C(r)}{c_C^*} + \frac{D_Q c_Q(r)}{D_C c_C^*} = 1 \tag{11}$$

The current for steady-state condition can be given as [13]:

$$\frac{I}{nF} = 2\pi\, L\, r_0\, D_Q \left(\frac{dc_Q}{dr}\right)_{r=r_0} \tag{12}$$

2.1. Normalised Form

By defining the following dimensionless variables

$$C = \frac{c_C}{c_C^*}, Q = \frac{c_Q}{c_C^*}, R = \frac{r}{r_0} \tag{13}$$

where C and Q are the dimensionless concentration of the catechol and o-quinone. R is the dimensionless distance parameter. The non-linear Equations (8-9) becomes in dimensionless form as follows:

$$\frac{d^2C}{dR^2} + \frac{1}{R}\frac{dC}{dR} - \frac{\gamma_E C}{1+\alpha C} = 0 \tag{14}$$

$$\frac{d^2\,Q}{dR^2} + \frac{1}{R}\frac{dQ}{dR} + \frac{\gamma_S C}{1+\alpha C} = 0 \tag{15}$$

where the dimensionless reaction-diffusion and saturation parameters [13] are

$$\alpha = \frac{c_C^*}{K_M}, \gamma_E = \frac{k_{cat} c_E r_0^2}{D_C K_M}, \gamma_S = \frac{k_{cat} c_E r_0^2}{D_Q K_M}, \frac{D_Q}{D_C} = \frac{\gamma_E}{\gamma_S}$$

The boundary conditions reduces as follows:

$$C = 1\,,\quad Q = 0 \quad \text{when} \quad R = 1 \tag{16}$$

$$C = 1\,,\quad Q = 0 \quad \text{when} \quad R = \frac{r_1}{r_0} \tag{17}$$

The dimensionless current at the micro-cylinder electrode is

$$\psi = I/n\,F L\, D_Q\, c_C^* = 2\pi\, \left(dQ/dR\right)_{R=1} \tag{18}$$

3. Analytical Solution of the Concentration Using NHPM

The NHPM yields solutions in convergent series form with easily computable terms, and in some cases, yields exact solutions in one iteration. In the present paper, the system of BVPs will be solved by the NHPM which is introduced by Aminikhah and Hemmatnezhad [16]. Using new approach of homotopy perturbation method, the dimensionless concentration is obtained as follows (Appendix A):

$$C_0(R) = \frac{e^{-\sqrt{\frac{\gamma_E}{1+\alpha}}\,R}\left(e^{\sqrt{\frac{\gamma_E}{1+\alpha}}\left(\frac{r_1}{r_0}+1\right)} + e^{2\sqrt{\frac{\gamma_E}{1+\alpha}}\,R}\right)}{e^{\sqrt{\frac{\gamma_E}{1+\alpha}}\,\frac{r_1}{r_0}} + e^{\sqrt{\frac{\gamma_E}{1+\alpha}}}} \tag{19}$$

And by adding the equations (14) and (15) and integrating with boundary conditions (16-17), we will have.

$$Q(R) = \frac{\gamma_E}{\gamma_S}(1 - C(R)) \tag{20}$$

The Equations (19) and (20) satisfy the boundary conditions (16) and (17). These equations represent the new and simple analytical expression of the concentration of catechol and o-quinone for all possible values of the parameters γ_E, γ_S, α and R From Equations (19) and (20), we can obtain the dimensionless current, which is as follows:

$$\psi = I/n\,F L\,D_Q\,c_C^* = 2\pi \left(\frac{e^{\sqrt{\frac{\gamma_E}{1+\alpha}}\left(\frac{r_1}{r_0}\right)} - e^{\sqrt{\frac{\gamma_E}{1+\alpha}}}}{e^{\sqrt{\frac{\gamma_E}{1+\alpha}}\,\frac{r_1}{r_0}} + e^{\sqrt{\frac{\gamma_E}{1+\alpha}}}} \right) \frac{\gamma_E}{\gamma_S}\sqrt{\frac{\gamma_E}{1+\alpha}} \tag{21}$$

4. Numerical Simulation

The non-linear differential equations (14) and (15) are solved using numerical methods. The function pdex2 in Scilab software which is the function of solving the boundary value problems for ordinary differential is used to solve this equation. Our theoretical results for the concentration of c_C using equation (19) and $c_E$using equation (20) are compared with simulation results (Scilab program 4.1) in Figures 1-2. The Scilab program is also given in Appendix B. Satisfactory agreement is found for all values of R.

5. Discussion

Figure 1 shows that the dimensionless concentration profile of catechol $C(R)$ using Equation (19) for all various values of the parameters γ_{E} andα. The plot was constructed for $r_1/r_0 = 1.5$ and 2.5. Thus it is concluded that there is a simultaneous increase in the values of the concentration of catechol as well as in saturated parameter α for small values of γ_{E}. Also the value of catechol concentration is uniform when γ_{E} is small and α is large. Figure 2 shows the concentration profile of O-quinone in R space for various values of γ_S, γ_E and α calculated using Equation (20). The plot was constructed for $r_1/r_0 = 1.5$. From the Figure 2 (a-c), we can observed that the dimensionless concentration of catechol should vary between 0 and 1. Because catechol is converted to $o-$quinone, the $o-$ quinone concentration should be the inverse of catechol. From Figure 2 it is observed that the concentration of quinone increases steadily and attain the maximum value then conclude decreases slowly. The concentration is maximum when $R = 1.25$ for all values of γ_S, γ_E and α whereas the concentration of catechol is minimum at $R = 1.25$. The dimensionless current ψ versus r_1/r_0 using Equation (21) is plotted in Figure 3. The value of current ψ increases when thickness of the film r_1/r_0 and dimensionless reaction-diffusion parameter γ_S is increases whereas the value of current ψ increases for the decreasing values of γ_E and α and current reaches the steady state value when $r_1/r_0 \geq 5$.

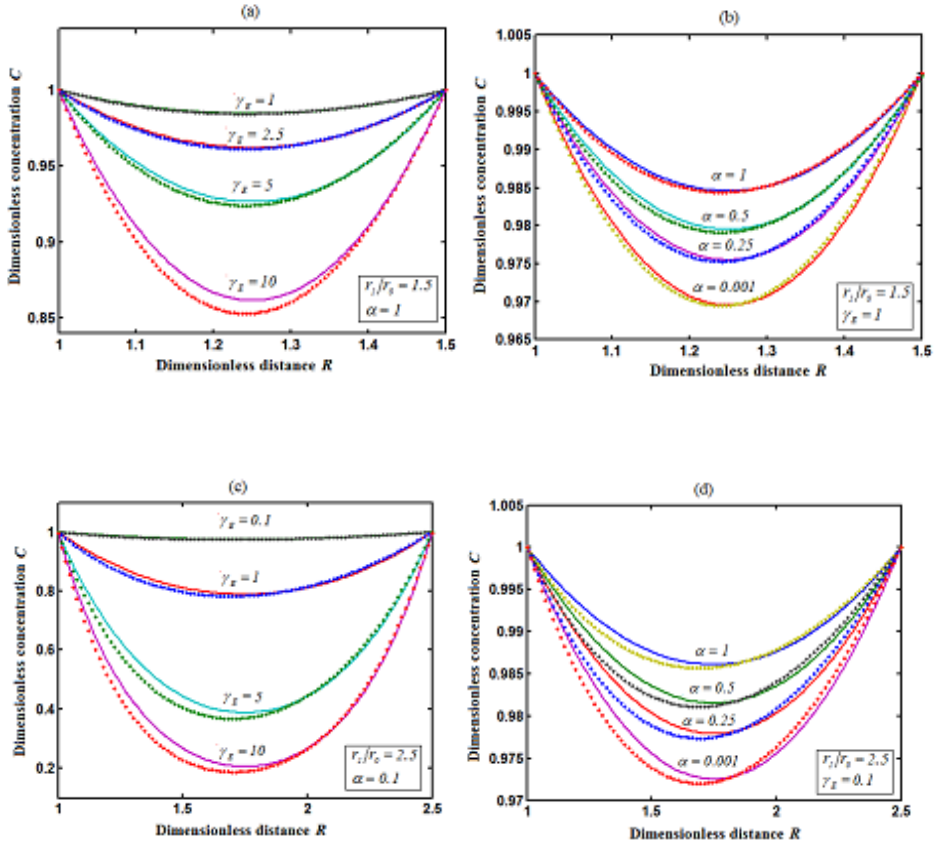

Figure 1(a-d): Dimensionless steady-state concentration profile of catechol $C\,(R)$ plotted from Equation (19). Figure 1 (a-b) for different values of parameters γ_E and α when $r_1/r_0 = 1.5$. Figure 1(c-d) for different values of parameters γ_E and α when $r_1/r_0 = 2.5$. Key to the graph: (___) represents the Equation (19) and (....) represents the numerical results.

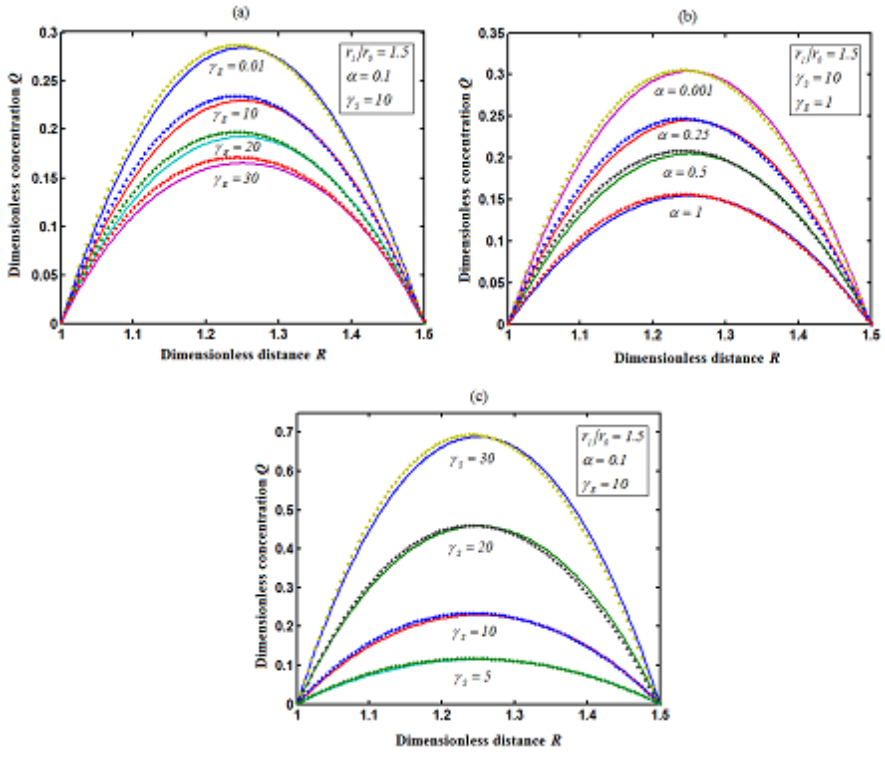

Figure 2(a-c) Dimensionless steady-state concentration profile of O-quinone $Q\,(R)$ plotted from Equation (20) for different values of parameters γ_E, α and γ_S when $r_1/r_0 = 1.5$. Key to the graph: (___) represents the Equation (20) and (....)

represents the numerical results.

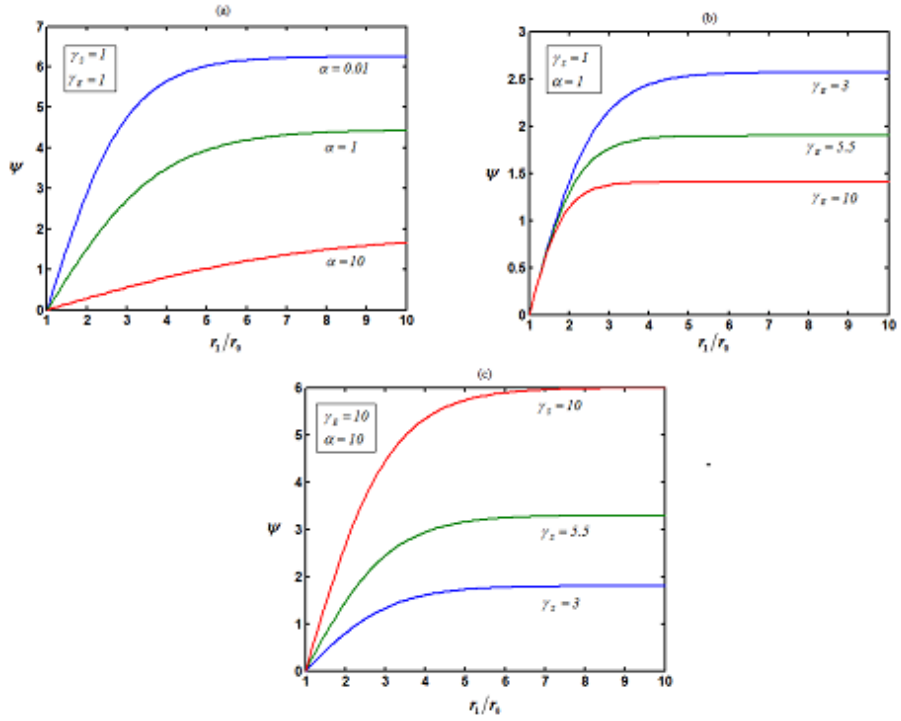

Figure 3. Plot of dimensionless current ψ versus r_1/r_0 for various values of parameters γ_E, α and γ_S. Current is calculated in the Equation (21).

6. Conclusions

The system of nonlinear time independent ordinary differential equation has been solved analytically using new Homotopy perturbation method. In this paper we have presented approximate analytical expression for the concentration of catechol and *o*- quinone. The primary result of this work is simple approximate calculation of concentration of catechol, *o*-quinone and current for all values of parameters. Analytical results are compared with simulation results and satisfactory agreement is noted.

Appendix A

Solution of the Equation (14) using new approach of homotopy perturbation method

In this appendix, we indicate how Equation (19) is derived. Furthermore, a homotopy was constructed to determine the solution of Equation (14) us follows:

$$(1-p)\left[\frac{d^2C}{dR^2} - \frac{\gamma_E C}{1+\alpha C\,(R=0)}\right] + p\left[(1+\alpha C)\left(\frac{d^2C}{dR^2} + \frac{1}{R}\frac{dC}{dR}\right) - \gamma_E C\right] = 0 \tag{A1}$$

The boundary conditions are as follows:

$$R = 0, \, , \, C = 1 \tag{A2}$$

$$R = \frac{r_1}{r_0}, \; C = 1 \tag{A3}$$

The approximate solutions of (A1) is

$$C = C_0 + pC_1 + p^2C_2 + p^3C_3 + \ldots \tag{A4}$$

Substituting Equation (A4) in Equation (A1) and comparing the coefficients of like powers of p

$$p^0 : \frac{d^2C_0}{dR^2} - \frac{\gamma_E C_0}{1+\alpha} = 0 \tag{A5}$$

The initial approximations are as follows:

$$R = 1,\ C_0 = 1 \tag{A6}$$

$$R = \frac{r_1}{r_0},\ C_0 = 1 \tag{A7}$$

Solving the Equation (A5) using the boundary conditions (A6) and (A7), we can find the following results

$$C_0(R) = \frac{e^{-\sqrt{\frac{\gamma_E}{1+\alpha}}\,R}\left(e^{\sqrt{\frac{\gamma_E}{1+\alpha}}\left(\frac{r_1}{r_0}+1\right)} + e^{2\sqrt{\frac{\gamma_E}{1+\alpha}}\,R}\right)}{e^{\sqrt{\frac{\gamma_E}{1+\alpha}}\,\frac{r_1}{r_0}} + e^{\sqrt{\frac{\gamma_E}{1+\alpha}}}} \tag{A8}$$

According to the HPM, we can conclude that

$$C(R) = \lim_{p\to 1} C(R) \cong C_0. \tag{A9}$$

Appendix B

Scilab program to find the numerical solution of the Equations (19-20)

```
function pdex2
m = 0;
x = linspace(1,2);
t=linspace(0,1000000);
sol = pdepe(m,@pdex2pde,@pdex2ic,@pdex2bc,x,t);
u1 = sol(:,:,1);
u2 = sol(:,:,2);
%-------------------------------------------------------
figure
plot(x,u1(end,:))
title('u1(x,t)')
xlabel('Distance x')
ylabel('u1(x,1)')
%-------------------------------------------------------
%figure
%plot(x,u2(end,:))
title('u2(x,t)')
xlabel('Distance x')
ylabel('u2(x,2)')
%-------------------------------------------------------
function [c,f,s] = pdex2pde(x,t,u,DuDx)
```

```
c = [1; 1];
f = [1; 1].*DuDx;
b=0.5;
g=1;
l=1;
F= (- g*u(1))*((1+u(1)*b)^(-1));
F1=(+ l*u(1))*((1+u(1)*b)^(-1));
s=[F; F1];
% ------------------------------------------------
function u0 = pdex2ic(x);
u0 = [1; 0];
% ------------------------------------------------
function [pl,ql,pr,qr]=pdex2bc(xl,ul,xr,ur,t)
pl = [ul(1)-1; ul(2)];
ql = [0; 0];
pr = [ur(1)-1; ur(2)];
qr = [0; 0];
```

Appendix C

Symbol	Definitions	Units
c_C	Concentration profile of catechol	mole/cm^3
c_E	Concentration profile of enzyme	mole/cm^3
c_Q	Concentration profile of quinine	mole/cm^3
D_C	Diffusion coefficient of catechol	cm^2/s
D_Q	Diffusion coefficient of quinine	cm^2/s
K_M	Michaelis Menten constant	mole/cm^3
K_{cat}	Catalytic rate constant	sec^{-1}
c_C^*	Bulk concentration of C	mole/cm^3
r	Radius of the cylinder	Cm
I	Current	Ampere
r_0	Electrode radius	Cm
r_1	Film radius	Cm
r_1/r_0	Dimensionless parameter for film thickness	None
χr_0	Dimensionless parameter for enzyme kinetic	None
j	Dimensionless sensor response	None
ψ	Dimensionless current	None
C	Dimensionless concentration of catechol	None
Q	Dimensionless concentration of quinine	None
R	Dimensionless distance	None
γ_E	Dimensionless reaction diffusion parameter	None
γ_S	Dimensionless reaction diffusion parameter	None
α	Dimensionless saturation parameter	None
L	Length of the electrode	Cm
F	Faraday constant	C mole^{-1}
n	Number of electrons	None

Table 1. **Nomenclature**

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