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Mathematical model of steady-state countercurrent bed-shrinking reactor in dilute acid

Saranya Jaganathan [1] and Rajendran Lakshmanan [2,*]

[1] *Research Scholar, Department of Mathematics, Mother Teresa Women's University, Kodaikanal–624 101, Tamil Nadu, India.*
[2] *Department of Mathematics, AMET (Deemed to be University), Kanathur, Chennai – 603 112, Tamil Nadu, India.*

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Abstract

The mathematical model of bed-shrinking in a countercurrent reactor proposed by Lee (Bioresource Technology 71 (2000) 29 - 39) is explored. This model is based on system of nonlinear differential equations. Analytically, the coupled nonlinear rate equations are solved. To produce approximate analytical expressions for hemicelluloses, oligomers, and xylose concentrations for all the values of non-dimensional parameters β, ω, and λ, the homotopy perturbation technique is applied. Our analytical results were compared to existing experimental data and found to be very similar. The dilute-acid pretreatment/hydrolysis of lignocellulosic biomass is studied using this mathematical model in the reactor.

Keywords: Mathematical modeling; Homotopy perturbation method; Lignocellulosic biomass; Nonlinear differential equations.

1. Introduction

Lignocellulose, sometimes called lignocellulosic biomass, is the dry matter (biomass) of plants. It is the world's most common required material for the creation of biofuels and bio-ethanol. This substance is made up of carbohydrate polymers (cellulose, hemicellulose) and an aromatic polymer. In dilute-acid lignocellulosic biomass, Lee et al. [1] created a mathematical model of a countercurrent shrinking-bed reactor. Rongfuchen et al. [2] established a mathematical model for dilute-acid hydrolysis of lignocellulosic biomass using a shrinking-bed reactor. Song et al. [3, 4] addressed the countercurrent reactor in lignocellulosic biomass acid saccharification. Song and Lee, as well as Greenwald et al. [5], devised a countercurrent reactor that produced high yields and sugar concentrations.

To the best of our knowledge, no analytical findings for the concentration of hemicelluloses, oligomer, and xylose at steady-state for all conceivable parameter values were available. We offer a novel approximate analytical result of concentrations for all parameter values in this investigation.

2. Mathematical Formulation of the Problem

The procedure for reacting of the dilute-acid hydrolysis of hemicelluloses model can be shown in [1]. The reaction is

$$H \xrightarrow{k_H} O \xrightarrow{k_3} X \xrightarrow{k_4} D, \tag{1}$$

* Corresponding author: Rajendran L
Department of Mathematics, AMET (Deemed to be University), Kanathur, Chennai – 603 112, Tamil Nadu, India.

where $k_H = F * k_1 + (1-F) * k_2$ and F is the fraction of the fast - hydrolyzed hemicelluloses portion. The following differential equations are expressed based on the total amount of solid material and hemicellulose (H) material.

$$\rho(1-\varepsilon)\frac{dv}{dx} - f\, K_H C_H = 0 \tag{2}$$

$$\frac{d(vC_H)}{dx} - K_H C_H = 0 \tag{3}$$

with respect to boundary conditions:

$$x = L \quad v = v_0 \tag{4}$$

$$x = L \quad C_H = C_{H0} \tag{5}$$

where ε is the voidage in the bed; ρ is the feedstock's solid density; and f is the ratio of total mass solubilized over hemicelluloses solubilized during the hydrolysis. The hemicellulose content in the solid (C_H) is defined on the basis of the reactor volume.

The following is the material balance for oligomer (O) and xylose (X) in the liquid stream:

$$\varepsilon u \frac{dC_0}{dx} - k_H C_H + \varepsilon k_3 C_0 = 0 \tag{6}$$

$$\frac{dC_X}{dx} - k_3 C_0 + k_4 C_X = 0 \tag{7}$$

with the following boundary conditions

At $x = 0$, $C_0 = 0$ (8)

At $x = 0$, $C_X = 0$ (9)

The dimensionless form of hemicelluloses, oligomer, and xylose concentration is presented below:

$$\frac{dY_H}{dZ} = \frac{\beta\omega}{\lambda(\lambda-1)}\left(Y^3{}_H - 2\lambda {Y_H}^2 + \lambda^2 Y_H\right) \tag{10}$$

$$\frac{dY_O}{dZ} = \frac{\beta}{\omega} Y_H - \beta\alpha_3 Y_O \tag{11}$$

$$\frac{dY_X}{dZ} = \beta\alpha_3 Y_O - \beta\alpha_4 Y_X \tag{12}$$

with respect to boundary conditions:

At $Z = 1$, $Y_H = 1$ (13)

At $Z = 0$, $Y_O = 0$ (14)

At $Z = 0$, $Y_X = 0$ (15)

The shrinkage factor (q) is the ratio of linear velocity of solid (v) at any point in the reactor to the initial linear solid feeding velocity (v_0). The hemicellulose content (Y_H) determines the shrinkage factor in solids.

$$q(z) = \frac{v}{v_0} = \frac{\lambda - 1}{\lambda - Y_H(z)} \tag{16}$$

where $\lambda = \rho(1-\varepsilon) / fC_{H_0}$ (17)

3. Approximate analytical expression steady-state concentration of hemicelluloses, oligomer and xylose using homotopy perturbation method (HPM)

Eqs (9–10) are used to represent the nonlinear equations. Finding an exact solution to these nonlinear equations is difficult. Nonlinear equations are notoriously difficult to solve, especially in a variety of scientific and technical contexts. A number of approximate analytical approaches [6], such as the homotopy perturbation method [7-11], the residual method [12], the Taylor series method [13–16], the AGM method [17–19], and a novel analytical method [20–22], have recently been used to solve the nonlinear equation. In this study, the homotopy perturbation approach is utilised to discover solutions to the nonlinear equations (9) - (10).

In physical chemistry and biology nonlinear phenomena are extremely important. Constructing a specific, accurate solution for these equations is still a challenge.Finding a specific, accurate solution for these equations is still a challenge. It is critical to find a precise solution with a physicochemical or biological interpretation. Ji-Huan was the first to introduce the HPM, which has subsequently been utilised to solve various nonlinear differential equations of various branches in mathematics and chemical science [23]. It is very powerful and novel method to obtain highly accurate solutions that are valid across the whole solution domain. Using this approach (see Appendix B), the following expression for the concentration of hemicelluloses, oligomer and xylose can be obtained:

$$Y_{\mathrm{H}}(z) = e^{-l\lambda^2(1-z)} + \frac{1}{2\lambda^2}\left[e^{l\lambda^2(z-1)}\right]\left[e^{l\lambda^2(z-1)} - 1\right]\left[e^{l\lambda^2(z-1)} - 4\lambda + 1\right] \tag{18}$$

$$\begin{aligned} Y_{\mathrm{O}}(z) = &\left[\frac{me^{-\lambda^2 l}}{\lambda^2 l + n} + \frac{2me^{-\lambda^2 l}}{\lambda(\lambda^2 l + n)} - \frac{me^{-\lambda^2 l}}{2\lambda^2(\lambda^2 l + n)}\right]\left[e^{\lambda^2 lz} - e^{-nz}\right] + \\ &\frac{2me^{-2\lambda^2 l}}{\lambda(2\lambda^2 l + n)}\left[e^{-nz} - e^{2\lambda^2 lz}\right] + \frac{me^{-3\lambda^2 l}}{2\lambda^2(3\lambda^2 l + n)}\left[e^{3\lambda^2 lz} - e^{-nz}\right] \end{aligned} \tag{19}$$

$$\begin{aligned} Y_{\mathrm{X}}(z) = &\frac{nm_0}{\beta\alpha_4 - n}\left[e^{(\beta\alpha_4 - n)z} - 1\right] + \frac{mm_1 e^{-\lambda^2 l}}{\beta\alpha_4 + \lambda^2 l}\left[1 - e^{z\left(\beta\alpha_4 + \lambda^2 l\right)}\right] + \\ &\frac{mm_2 e^{-2\lambda^2 l}}{\beta\alpha_4 + 2\lambda^2 l}\left[e^{z\left(\beta\alpha_4 + 2\lambda^2 l\right)} - 1\right] + \frac{mm_3 e^{-3\lambda^2 l}}{\beta\alpha_4 + 3\lambda^2 l}\left[1 - e^{z\left(\beta\alpha_4 + 3\lambda^2 l\right)}\right] \end{aligned} \tag{20}$$

where

$$l = \frac{\beta\omega}{\lambda(\lambda-1)},\ m = \frac{\beta}{\omega},\ n = \beta\alpha_3,$$

$$m_0 = \frac{-me^{-\lambda^2 l}}{\lambda^2 l + n} - \frac{2me^{-\lambda^2 l}}{\lambda(\lambda^2 l + n)} + \frac{me^{-\lambda^2 l}}{2\lambda^2(\lambda^2 l + n)} + \frac{2me^{-2\lambda^2 l}}{\lambda(2\lambda^2 l + n)} - \frac{me^{-3\lambda^2 l}}{2\lambda^2(3\lambda^2 l + n)} \tag{21}$$

$$m_1 = \frac{2\lambda^2 + 4\lambda - 1}{2\lambda^2(\lambda^2 l + n)},\ m_2 = \frac{2}{\lambda(2\lambda^2 l + n)} \text{ and } m_3 = \frac{1}{2\lambda^2(3\lambda^2 l + n)}$$

4. Results and discussion

Eqs. (18) to (20) represent the simple analytical expressions pertaining to the dimensionless concentration of hemicelluloses in solid, oligomer in liquid and xylose in liquid for all values of dimensionless parameters β, ω, and λ. It is interesting to see how each parameter affects the concentration of hemicelluloses, oligomers, and xylose for different parameter values.

The kinetic pattern of lignocellulosic biomass dilute-acid hydrolysis is dependent on the substrate concentration. The concentration of the substrate, on the other hand, is determined by dimensionless parameter β, ω, and λ .The dimensionless parameter β is determined by the hemicellulose hydrolysis rate constant, reactor length, and liquid linear velocity. The dimensionless parameter ω depends upon liquid linear velocity and initial linear solid feeding velocity. The parameter λ is proportional to solid density, void fraction in bed, percentage of hemicelluloses content in original biomass and ratio of solubilized biomass to solubilized hemicelluloses (or cellulose).

The dimensionless concentration of hemicelluloses Y_H versus Z for different values of β, ω and λ is depicted in Figures 1(a) - 1(c). From Figures 1(a) - 1(c), it is inferred that the concentration of hemicelluloses decreases when β, ω and λ increases for some fixed values of other parameters.

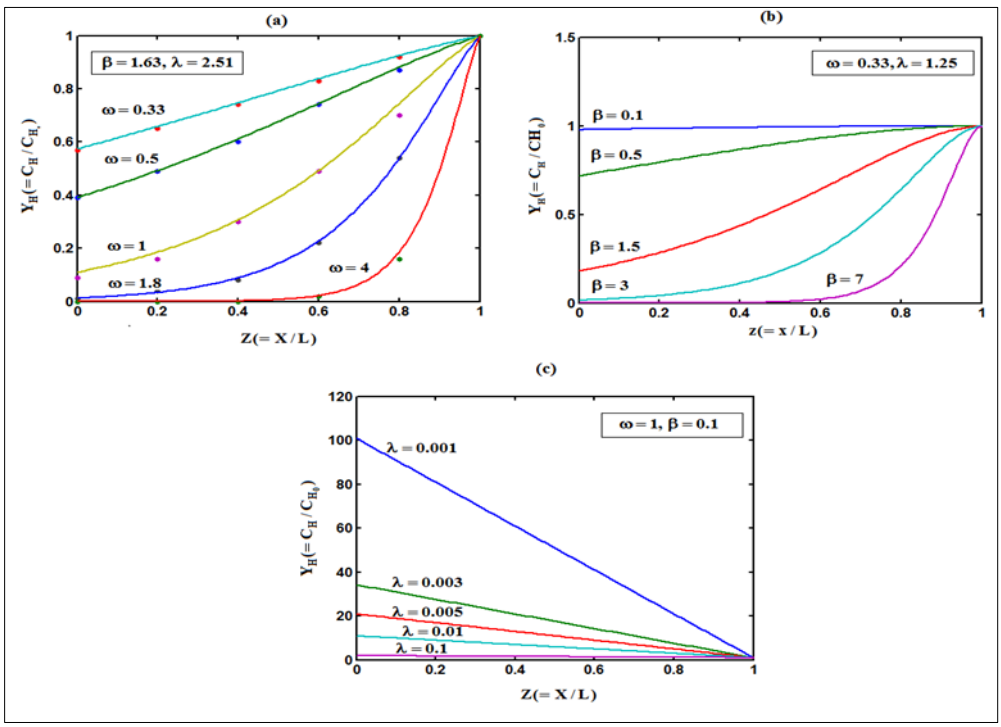

Figure 1 Comparison of steady-state concentration of hemicelluloses using Eq. (10) for (a) different values of ω with experimental results [1], (b) for different values of β (c) for different values of λ.

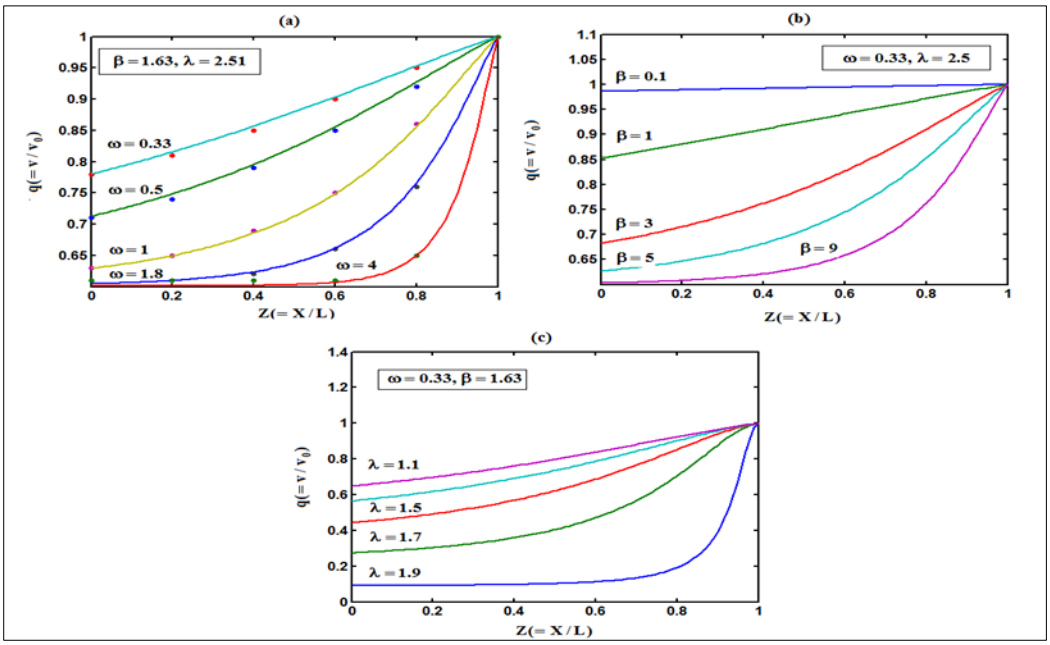

Figure 2 (a) Comparison of normalized steady- state bed shrinking factor q versus distance z using Eq.(16) (a) for different values of ω with experimental results[1]. **(b)** for different values of β . **(c)** for different values of λ

In Figures 2(a)-2(c), the shrinking factor q versus Z for different values of parameters are plotted. From these figures it is observed that the shrinking factor decreases when β, ω , and λ increases for some fixed values of other parameters.

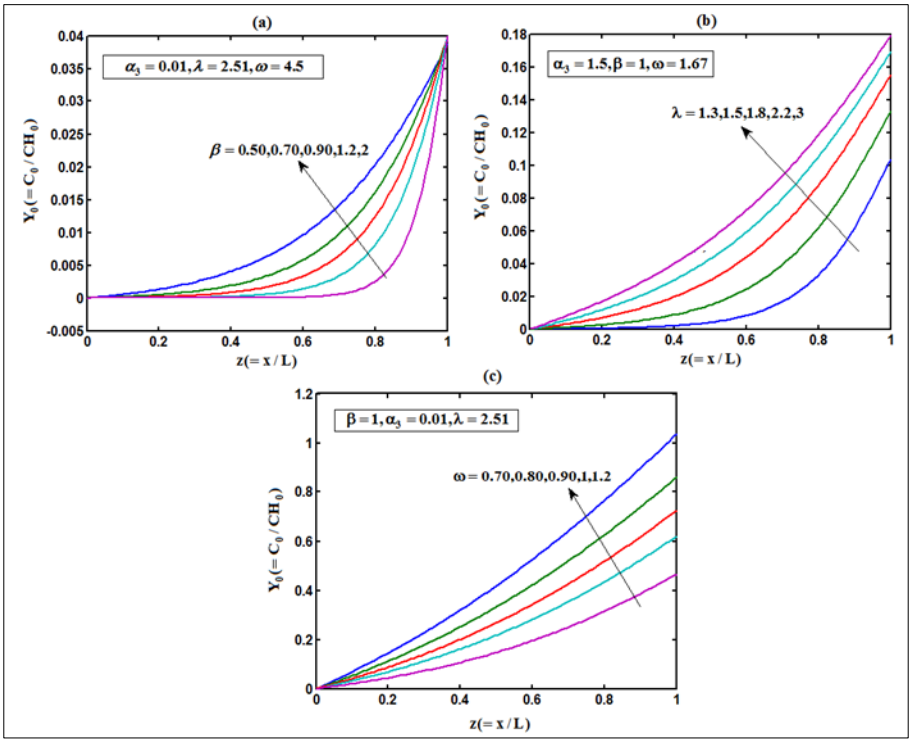

Figure 3 (a) Comparison of steady-state concentration of oligomer using Eq. (11) for different values of β with experimental result [1]. **(b)** for different values of λ . **(c)** for different values of ω .

In Figures 3(a) - 3(c), the concentration of oligomer in liquid Y_O versusZ for different values of parameters are plotted. From these figures it is deduced that the concentration of oligomer increases when $\beta, \omega,$ and λ increases for some fixed values of other parameters.

In Figures 4(a) - 4(e), the concentration of xylose in liquid Y_X versus Z for different values of parameters are plotted. When $\beta, \alpha_3, \alpha_4, \lambda$ and ω increases for some fixed values of other parameters, concentration of xylose increases.

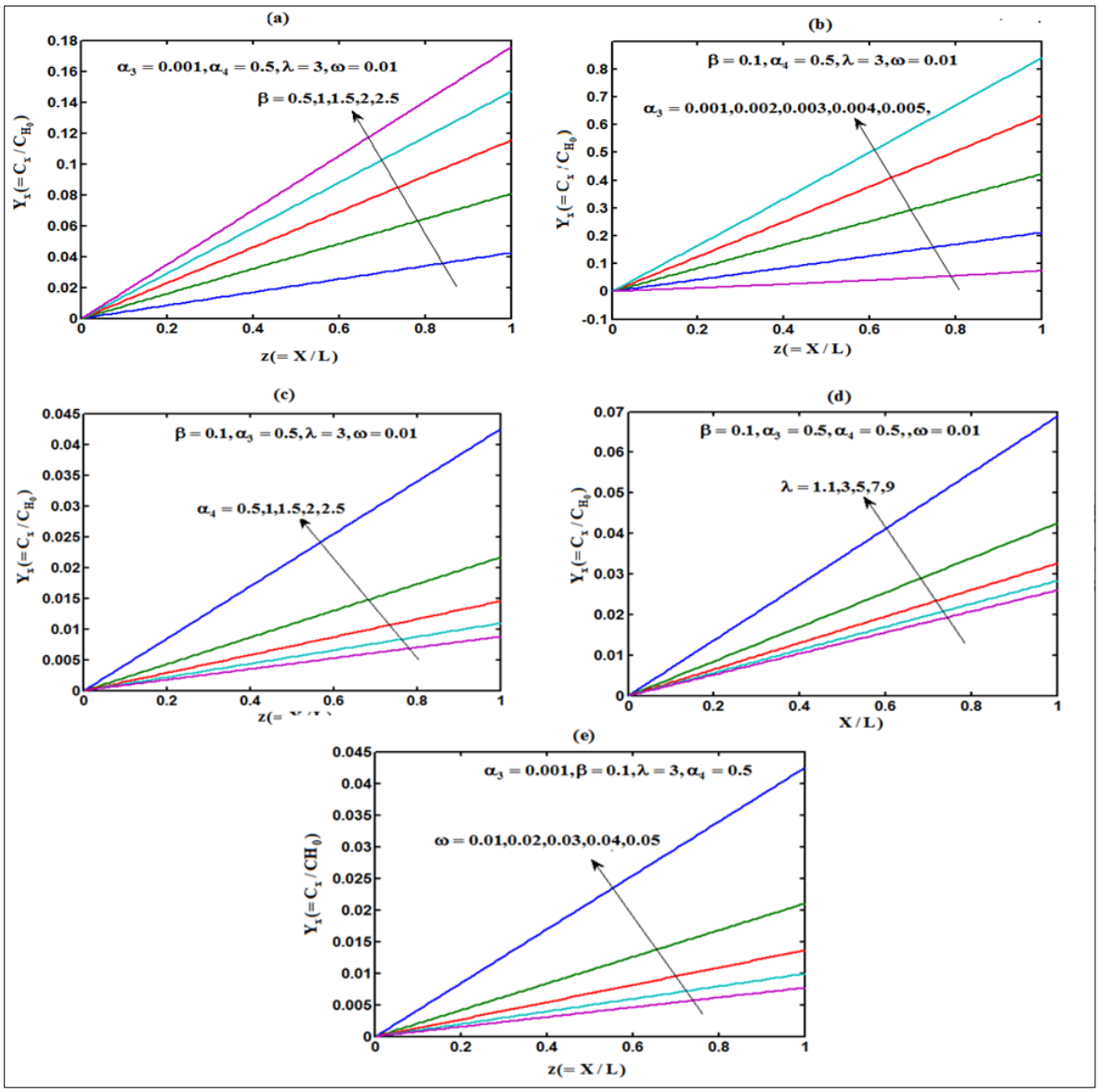

Figure 4 (a) Comparison of steady-state concentration of xylose using Eq.(12) (a) for different values of β with experimental result [1]. **(b)** for different values of α_3. **(c)** for different values of α_4. (d) for different values of λ. (e) for different values of ω.

The solid feeding velocity, linear liquid velocity, temperature, sulphuric acid concentration, and bed shrinking are the process factors investigated in this study. The output parameters of reactor performance are sugar concentration, yields, and reactor processing capacity.

5. Conclusion

We present a theoretical model that describes the behaviour of a continuous countercurrent shrinking-bed reactor in this study. With the use of homotopy perturbation techniques, a nonlinear time independent problem was solved analytically. Approximate analytical expressions for the concentrations of the substrate and products are derived. This approach is both easy to use and promising for solving the non-linear equations. The purpose of this model is to provide a foundation for designing and operating this unique reactor system.

6. Appendix A

6.1. Basic concepts of the HPM

The core principle of the HPM is presented in this appendix. This method has overcome the constraints of classic perturbation methods. However, because it can fully use traditional perturbation approaches, there has been a significant amount of study to solve a variety of severely nonlinear equations. The following function is used to describe this method:

$$A(u) - f(r) = 0 \qquad r \in \Omega \tag{A1}$$

With the following boundary conditions:

$$B\left(u, \frac{\partial u}{\partial n}\right) = 0, \qquad r \in \Gamma \tag{A2}$$

where A, B, f(r) and Γ respectively, indicate a generic differential operator, a boundary operator, a known analytical function, and the domain boundary Ω. The operator A may be split into two parts: a linear portion L and a non-linear part N. As a result, Eq. (A1) may be rewritten as

$$L(u) + N(u) - f(r) = 0 \tag{A3}$$

Using the homotopy method, a homotopy $v(r,\mathrm{p}): \Omega \times [0,1] \to R$ is built in such a way that

$$H(v,\mathrm{p}) = (1-\mathrm{p})[L(v) - L(u_0)] + \mathrm{p}[A(v) - f(r)] = 0 \tag{A4}$$

$$\mathrm{p} \in [0,1], \qquad r \in \Omega \tag{A5}$$

where $\mathrm{p} \in [0,1]$ is an embedding parameter or homotopy parameter and is an initial approximation of Eq.(A1), that meets the boundary requirements. Eqs. (A4) and (A5) may obviously be deduced to provide (A6) and (A7).

$$H(v,0) = L(v) - L(u_0) = 0 \tag{A6}$$

$$H(v,1) = A(v) - f(r) = 0 \tag{A7}$$

Eq. (A4) or (A5) forms a linear equation when $\mathrm{p} = 0$, and a nonlinear equation when $\mathrm{p} = 1$. As a result, the process of moving p from zero to unity is identical to that of. To begin, the embedding parameter p can be considered to be a tiny parameter, and the solutions of Eqs. (A4) and (A5) can be expressed as a power series of p:

$$v = v_0 + \mathrm{p}v_1 + \mathrm{p}v_2 + \ldots\ldots \tag{A8}$$

when $p = 1$ is used, the following is the approximate solution to Eq. (A1): $u = \lim_{p \to 1} v = v_0 + v_1 + v_2 + \ldots\ldots$

(A9)

The homotopy perturbation technique is the result of combining the perturbation method and the homotopy method.

6.2. Appendix B

6.2.1. Approximate analytical solutions of the Eqn (10) using the HPM.

To get the solution to Eq. (10), first create the homotopy as follows:

$$(1-\mathrm{p})\left[\frac{d\mathrm{Y_H}}{dz}-A\lambda^2\mathrm{Y_H}\right]+\mathrm{p}\left[\frac{d\mathrm{Y_H}}{dz}-A\lambda^2\mathrm{Y_H}-A\mathrm{Y_H^3}+2A\lambda\mathrm{Y_H^2}\right]=0 \quad \text{(B1)}$$

Eq. (B1) has the following approximate solution:

$$Y_{\mathrm{H}}=Y_{H0}+\mathrm{p}Y_{H1}+\mathrm{p}^2Y_{H2}+..... \quad \text{(B2)}$$

When Eq. (B2) is substituted in Eq. (B1), the outcome is:

$$\begin{aligned}&(1-p)\left[\frac{d\left(Y_{H0}+\mathrm{p}Y_{H1}+\mathrm{p}^2Y_{H2}+.....\right)}{dz}-A\lambda^2\left(Y_{H0}+\mathrm{p}Y_{H1}+\mathrm{p}^2Y_{H2}+.....\right)\right]+\\&p\left[\begin{array}{l}\dfrac{d\left(Y_{H0}+\mathrm{p}Y_{H1}+\mathrm{p}^2Y_{H2}+.....\right)}{dz}-A\lambda^2\left(Y_{H0}+\mathrm{p}Y_{H1}+\mathrm{p}^2Y_{H2}+.....\right)\\-A\left(Y_{H0}+\mathrm{p}Y_{H1}+\mathrm{p}^2Y_{H2}+.....\right)^3+2A\lambda\left(Y_{H0}+\mathrm{p}Y_{H1}+\mathrm{p}^2Y_{H2}+.....\right)^2\end{array}\right]=0\end{aligned} \quad \text{(B3)}$$

The coefficients of similar powers of p are compared:

$$\mathrm{p}^0:\quad \frac{dY_{H0}}{dz}-A\lambda^2Y_{H0}=0 \quad \text{(B4)}$$

$$\mathrm{p}^1:\ \frac{dY_{H1}}{dz}-A\lambda^2Y_{H1}-AY_{H0}^3+2\lambda AY_{H0}^2=0 \quad \text{(B5)}$$

Using the boundary conditions $Z=1,\ Y_{H_0}=1,\ Y_{H_1}=0,$ we can solve Eqs. (B4) and (B5). Solving the Eqs (B4) and (B5), we get the following result.

$$Y_{H0}(z)=e^{-A\lambda^2(1-z)} \quad \text{(B6)}$$

$$Y_{H1}(z)=\frac{1}{2\lambda^2}\left[e^{A\lambda^2(z-1)}\left[e^{A\lambda^2(z-1)}-1\right]\left[e^{A\lambda^2(z-1)}-4\lambda+1\right]\right] \quad \text{(B7)}$$

According to the HPM, the following may be concluded:

$$Y_{\mathrm{H}}=\lim_{p\to1}y\approx Y_{H0}(z)+Y_{H1}(z) \quad \text{(B8)}$$

The final findings can be represented in the text as Eq. (9) after combining Eqs. (B6) and (B7) in (B8). Similarly, we may derive Eq. (10) in the text by putting Eq. (9) into Eq. (7). Similarly we get Eq. (11) in the text after inserting Eq.(10) into Eq. (8).

6.3. Nomenclature

Symbols	Units	Definition
C_c	g/100 ml	Concentration of cellulose
C_{c_0}	g/100 ml	Initial concentration of cellulose
C_H	g/100 ml	Concentration of hemicelluloses in solid
C_{H_0}	g/100 ml	Initial concentration of hemicelluloses
C_0	g/100 ml	Concentration of oligomer
C_x	g/100 ml	Concentration of xylose
E_i	kcal/g mol	Activation energy for k_i
H	None	Hemicelluloses
H_1	None	Rapidly hydrolyzed hemicelluloses
H_2	None	Slowly hydrolyzedhemicelluloses
H_0	None	The percentage of hemicelluloses in the original biomass
$k_i = A^m k_{oi} \exp\left(-E_1/RT\right)$	min^{-1}	Hydrolysis of hemicelluloses rate constant
k_{oi}	$\min^{-1}(wt\%)^{-ni}$	Frequency factor for k_i
k_C, k_G	min^{-1}	Cellulose hydrolysis rate constant
k_H	min^{-1}	Rate constant
L	cm	Reactor length
n_i	None	Exponent of acid concentration
O	None	Hemicellulose oligomer
$q = \frac{v}{v_0}$	cm/min	Bed shrinking factor
R	$Jk^{-1}mol^{-1}$	Constant of universal gas
S	wt%	Concentration of acid
T	K	Temperature
u	cm/min	Linear velocity of liquid
v	cm/min	Linear velocity of Solid
v_0	cm/min	Initial linear solid feeding velocity
$v_{0,opt}$	cm/min	Optimal initial linear solid feeding velocity
W	(g biomass) / (min*(ml reactor volume))	Reactor processing capacity
X	g/100 ml	Xylose

$Y_H = \frac{C_H}{C_{H0}}, Y_o = \frac{C_o}{C_{H0}}, Y_X = \frac{C_X}{C_{H0}}$	None	Dimensionless concentration
Z=x/L	None	Dimensionless reactor length
$\alpha_3 = {}^{k_3}\!/_{k_1}, \alpha_4 = {}^{k_4}\!/_{k_1}$	None	Dimensionless rate constant
ε	None	Void fraction in bed 0.35
Y_H	None	Dimensionless concentration of hemicelluloses
Y_O,	None	Dimensionless concentration of oligomer
Y_x	None	Dimensionless concentration of xylose
$\beta = {}^{k_1 L}\!/_{u}$	None	Dimensionless parameters
$\lambda = \frac{\rho(1-\varepsilon)}{fH_0}$	None	Dimensionless parameters
$\omega = \frac{u}{v_0}$	None	Dimensionless parameters
l	None	Dimensionless parameters
m	None	Dimensionless parameters
n	None	Dimensionless parameters
m_0	None	Dimensionless parameters
m_1	None	Dimensionless parameters
m_2	None	Dimensionless parameters
m_3	None	Dimensionless parameters

Compliance with ethical standards

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Disclosure of conflict of interest

The author declares that they have no known competing financial interests or personal relationships that could have influenced the work reported in this paper.

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