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Development of a Model for the Process of Anaerobic Digestion and its Solution by the Modified Adomian Decomposition Method and a Simplified Runge-Kutta Method

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Abstract:

This term paper works on developing a mathematical model for the process of Anaerobic Digestion, that describes the transformation of biomass into biogas, and solving it to investigate the variation of concentration of various species that take part in the process. It attempts to solve the system of equations using the Modified Adomian Decomposition Method, a powerful technique used to solve systems of linear and non-linear differential equations, since it is computationally convenient, precise and physically realistic. Further, it also presents the results using the simplified second-order and fourth-order Runge-Kutta methods. By using the results obtained, we aim to replicate the data presented in the original research paper.

Keywords:

Anaerobic Digestion, Adomian Decomposition Method, Runge-Kutta Method, Kinetic System of ODE’s.

1. Introduction:

Anaerobic Digestion (AD) is a biochemical process for biogas production. Biogas is a fuel mainly composed of methane and carbon dioxide. In this process, it is formed from the biological degradation of biomass, the world's most abundant raw material that consists of substances of organic origin, such as plants, animals and microorganisms.

The paper ventures into the field of biogas production and modelling a solving method to predict the time required for the chemical process of AD to give out an optimum concentration. The motivation lies behind the fact that the pre-existing procedures are relatively inefficient, whereas we try to find the a suitably accurate prediction closest to the real world.

Anaerobic digestion is a complex process of metabolic interactions, taking place in the absence of oxygen and being performed by microbial populations. This mathematical modelling is based on the chemical reactions in the process and provides a set of coupled and non-linear ordinary differential equations

In this paper, a chemical and mathematical model of the AD process is developed, where cellulose is the substrate. In addition, we simulate this process by solving the system of ordinary differential equations using the Modified Adomian Decomposition method, applied to the time variable, and the Simplified Runge-Kutta methods of second-order and fourth-order.

The Adomian Decomposition Method (ADM) is an effective technique used to solve this problem, which involves non-linear terms in a series of polynomials. Some researchers have introduced modifications in the ADM technique. For example, Younker modified the ADM to solve a system of coupled differential equations describing chemical reaction rates.

Runge-Kutta Methods are iterative methods used in calculation of the solutions of Ordinary Differential Equations. These methods provide a high accuracy in the approximation of the solution, without having to calculate the higher order derivatives.

We attempt to code the ADM, the RK-2 and RK-4 methods, and utilize them to solve the system of equations and further compare the results obtained with the data presented in the original paper.

2. Chemical and Mathematical Modelling:

The Anaerobic Digestion process of Biomass takes place in multiple phases and steps. The reactions and few corresponding ΔG values of the anaerobic digestion process are :-

(I) Hydrolysis:

Complex organic compounds like sugars, proteins and fats are decomposed to form soluble monomers.

$$C_6H_{10}O_5 + H_2O \rightarrow C_6H_{12}O_6$$

(II) Acidogenesis:

Sugars fermented to predominantly form short chain acids, alcohols and ketones.

$$C_6\,H_{12}O_6 \rightarrow C_4H_8O_2 + 2H_2 + 2CO_2 \qquad , \Delta G = -\frac{264KJ}{mol}$$

(III) Acetogenesis:

Fermentation of carbohydrates takes place, products of lipid hydrolysis are oxidised to form acetates, propionate and gaseous hydrogen

$$2C_4H_8O_2 + 2H_2O + CO_2 \rightarrow CH_4 + 4C_2H_4O_2 \qquad , \Delta G = -\frac{35KJ}{mol}$$

(IV) Hydrogenotrophic methanogenesis:

Production of methane form hydrogen (as a reducing agent) and carbon dioxide(as a source for carbon)

$$4H_2 + CO_2 \rightarrow CH_4 + 2H_2O \qquad , \Delta G = -\frac{131KJ}{mol}$$

(V) Acetoclastic methanogenesis:

Production of methane form acetic acid or methanol by methanogenic archaea, which is also responsible for 70% of total methane production

$$C_2H_4O_2 \rightarrow CO_2 + CH_4 \qquad , \Delta G = -\frac{36KJ}{mol}$$

Chemical compounds	Chemical Formula	Abbreviations
Cellulose	$C_6H_{10}O_5$	Y_1
Glucose	$C_6H_{12}O_6$	Y_2
Butyric Acid	$C_4H_8O_2$	Y_3
Acetic Acid	$C_2H_4O_2$	Y_4
Methane	CH_4	Y_5
Carbon dioxide	CO_2	Y_6
Hydrogen	H_2	Y_7
Water	H_2O	Y_8

Table 1: Chemical compounds, formulas and their abbreviations

The kinetic system of differential equations according to the rate law analysis can be formulated as

$$\left.\begin{aligned}
\frac{dY_1}{dt} &= -k_0Y_1Y_8 && Y_1(0)=1\\
\frac{dY_2}{dt} &= k_0Y_1Y_8 - k_1Y_2 && Y_2(0)=0\\
\frac{dY_3}{dt} &= k_1Y_2 - k_2Y_3Y_8Y_6^{\frac{1}{2}} && Y_3(0)=0\\
\frac{dY_4}{dt} &= 2k_2Y_3Y_8Y_6^{\frac{1}{2}} - 2k_4Y_4^2 && Y_4(0)=0\\
\frac{dY_5}{dt} &= \frac{1}{2}k_2Y_3Y_8Y_6^{\frac{1}{2}} + \frac{1}{2}k_3Y_7^2Y_6^{\frac{1}{2}} + 2k_4Y_4^2 && Y_5(0)=0\\
\frac{dY_6}{dt} &= 2k_1Y_2 - \frac{1}{2}k_2Y_3Y_8Y_6^{\frac{1}{2}} - \frac{1}{2}k_3Y_7^2Y_6^{\frac{1}{2}} + 2k_4Y_4^2 && Y_6(0)=0\\
\frac{dY_7}{dt} &= 2k_1Y_2 - 2k_3Y_7^2Y_6^{\frac{1}{2}} && Y_7(0)=0\\
\frac{dY_8}{dt} &= -k_0Y_1Y_8 - k_2Y_3Y_8Y_6^{\frac{1}{2}} + k_3Y_7^2Y_6^{\frac{1}{2}} && Y_8(0)=1
\end{aligned}\right\} \quad (1)$$

Here Y_i values are the corresponding molar concentrations of the species and k_i is found by the ΔG values and the given relation

$$k_i = e^{\frac{-\Delta G}{RT}} \quad (2)$$

We assume $k_0 = 1$, and calculate the rate constants for the reactions considering the ambient temperature as T_i=298.15 K. The following values are obtained:

Parameter	**Value**
k_0	1
k_2	1.1125
k_2	1.014
k_3	1.054
k_4	1.015

Table 2: Values of k used in simulation

Starting with 1 mole of glucose as the substrate the final net chemical reaction obtained is:

$$C_6H_{12}O_6 = 3CH_4 + 3CO_2$$

3. Numerical Analysis:

In this section we present the details to find the solution of the problem formulated in *Section 2* first using the Runge-Kutta Methods and then by the Modified Adomian Decomposition Method.

3.1 Runge-Kutta Methods

(The notation 'k' generally used in RK Method has been modified to 'a' here to avoid confusion with the notation of rate constant used in this paper)

Runge-Kutta Methods are iterative methods used in calculation of the solutions of Ordinary Differential Equations. These methods provide a high accuracy in the approximation of the solution, without having to calculate the higher order derivatives.

The general form of the methods to solve an ODE of the form $\frac{dy}{dx} = f(x, y)$ is given by

$$y_{i+1} = y_i + \phi(x_i, y_i, h) \tag{3.1}$$

Where $\phi(x_i, y_i, h)$ is called the *increment function.* The general form of the increment function is

$$\phi = m_1 a_1 + m_2 a_2 + \cdots + m_n a_n \tag{3.2}$$

where, a's are constants and the k's are

$$a_1 = hf(x_i, y_i) \tag{3.3}$$
$$a_2 = hf(x_i + p_1 h,\ y_i + q_{11} k_1) \tag{3.4}$$
$$a_3 = hf(x_i + p_2 h,\ y_i + q_{21} a_1 + q_{22} a_2) \tag{3.5}$$

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$$a_n = hf\left(x_i + p_{n-1} h,\ y_i + q_{(n-1)1} a_1 + q_{(n-1)2} a_2 + \cdots + q_{(n-1)(n-1)} a_{(n-1)}\right) \tag{3.6}$$

where, p's and q's are constants for a given type of RK method. The recurrence relations between a_i's makes these RK Methods efficient for computational calculations.
In this paper we mainly focus on the RK Methods of the second and fourth order i.e. n=2 and n=4.

- <u>Second Order Runge-Kutta Method</u> :
  The Second-order RK method is the Eq. (3.1) written as

$$y_{i+1} = y_i + \frac{(a_1 + a_2)}{2} \tag{4.1}$$

where,

$$a_1 = hf(x_i, y_i) \tag{4.2}$$
$$a_2 = hf(x_i + h,\ y_i + a_1) \tag{4.3}$$

- <u>Fourth Order Runge-Kutta Method</u> :
  The Fourth-order RK method or the 'Classical RK method' is the Eq. (3.1) written as

$$y_{i+1} = y_i + \frac{1}{6}(a_1 + 3a_2 + 3a_3 + a_4) \tag{5.1}$$

where,

$$a_1 = hf(x_i, y_i) \tag{5.2}$$

$$a_2 = hf\left(x_i + \frac{h}{2},\ y_i + \frac{a_1}{2}\right) \tag{5.3}$$

$$a_3 = hf\left(x_i + \frac{h}{2},\ y_i + \frac{a_2}{2}\right) \tag{5.4}$$

$$a_4 = hf(x_i + h,\ y_i + a_3) \tag{5.5}$$

3.2 Adomian Decomposition Method

The Adomian Decomposition Method (ADM) is an effective technique used to solve this problem, which involves the writing of non-linear terms in a series of polynomials.

If the IVP for a First-Order system of equations of the following form

$$\left.\begin{array}{ll} y_1'(t) = f_1(t, y_1, \cdots, y_m)\,, & y_1(0) = y_{1,0} \\ y_2'(t) = f_2(t, y_1, \cdots, y_m), & y_2(0) = y_{2,0} \\ \cdot & \\ \cdot & \\ \cdot & \\ y_m'(t) = f_m(t, y_1, \cdots, y_m), & y_m(0) = y_{m,0} \end{array}\right\} \tag{6.1}$$

Where $f_k(t, y_1, \cdots, y_m), k = 1,2, \dots, m$ are linear and nonlinear functions

$$L_{y_k} = f_m(t, y_1, \cdots, y_m), k = 1,2, \dots, m \tag{6.2}$$

Where L is the linear operator (a time derivative)
The following method consists of segregating f_k into non-linear and linear part, transforming Eq(6) into

$$L_{y_k} = R_k(t, y_1 \cdots \cdots y_m) + N_k(t, y_1 \cdots \cdots y_m) \tag{7}$$

where $R_k(t, y_1 \cdots \cdots y_m)$ are linear operators and $N_k(t, y_1 \cdots \cdots y_m)$ are nonlinear

Introducing the inverse operator $L^{-1}(\cdot) = \int_0^t (\cdot)\, dt$ on both the sides of Eq (7) gives

$$y_k = y_0 + L^{-1}\{R_k(t, y_1 \cdots\cdots y_m) + N_k(t, y_1 \cdots\cdots y_m)\} \tag{8}$$

where $y_k(0)$ is the initial value condition of the problem

We seek the solution $\{y_1 \cdots\cdots y_m\}$ as

$$y_k = \lim_{n\to\infty} \sum_{i=0}^{n} y_{k,i} \tag{9}$$

The non-linear terms of $N_k(t, y_1 \cdots\cdots y_m), k = 1, \dots.m$ are assumed to be analytical functions that can be expressed by an infinite series given by

$$N_k(t, y_1 \cdots\cdots y_m) = \sum_{n=0}^{\infty} A_{k,n}\,,\ \ k = 1, \dots\dots m, \tag{10}$$

Where $A_{k,n}$ are Adomian polynomials calculated by the formula

$$A_{k,n} = \frac{1}{n!}\left[\frac{d^n}{d\lambda^n} N_k\left(t, \sum_{i=0}^{n} y_{k,i}\lambda^i\,, \sum_{i=0}^{n} \lambda^i y_{2,i}\,, \dots, \sum_{i=0}^{n} \lambda^i y_{m,i}\right)\right]_{\lambda=0} \tag{11}$$

at $\lambda = 0$

taken as per general method procedure seen throughout the *various* papers.

Taking the first n+1 terms of the n-th approximation of y_k

$$y_k = \sum_{i=0}^{n} y_{k,i} \tag{12}$$

And substituting Eq. (10) and (12) in (8) gives

$$y_k = y_k(0) + L^{-1}\left[R_k(t, y_1 \cdots\cdots y_m) + \sum_{i=0}^{n} A_{k,n}\,,\right] \tag{13}$$

$$k = 1, \dots\dots m,$$

The 1st term of this series is given by the formula

$$y_k(0) = y_{k,0}\ \ ,\quad k = \{1, \dots\dots m\}$$

$$y_{k,i+1} = L^{-1}\{R_k + A_{k,i}\}\ \ ,\quad k = \{1, \dots\dots m\}\ i = \{0, \dots\dots n\} \tag{14}$$

The final solution of the system is given by

$$y_k = y_{k,0} + y_{k,1} + \cdots + y_{k,n}\,,\qquad k = 1, \dots\dots m \tag{15}$$

Solution of the Problem:

3.3 By Runge-Kutta Methods

To solve the system of Ordinary Differential Equations modelled as Initial Value Problems in Eq. (1) using 2nd and 4th order RK methods, the step size is taken to be $h = 0.1\ days$. For the system of ODE's the Eq. (3.1) is applied to each separate ODE and the values of a_i are calculated for each equation separately.

- Second Order Runge-Kutta Method :
  For the kinetic system of ODE's given in Eq. (1), the RK method is modified to a vector equation to represent all the 8 ODE's as

$$\bar{Y}_{i+1} = \bar{Y}_i + \frac{(\bar{a}_1 + \bar{a}_2)}{2} \tag{16}$$

where, $\bar{Y}_i = [\, Y_{1_i} \;\; Y_{2_i} \;\; \cdots \;\; Y_{8_i} \,]$

$\bar{a}_i = [\, a_{i,1} \;\; a_{i,2} \;\; \cdots \;\; a_{i,8} \,]$ for the given set of 8 ODE's.

For each application of the second order RK method, the values of $\underline{a}_1$ & $\underline{a}_2$ are calculated for each equation as follows

Value of a_1

For Y_1

$$a_{1,1} = hf_1(t_i, \bar{Y}_i)$$
$$a_{1,1} = h(-k_0 Y_{1_i} Y_{8_i})$$

For Y_2

$$a_{1,2} = hf_2(t_i, \bar{Y}_i)$$
$$a_{1,2} = h(k_0 Y_{1_i} Y_{8_i} + k_1 Y_{2_i})$$

For Y_3

$$a_{1,3} = hf_3(t_i, \bar{Y}_i)$$
$$a_{1,3} = h(k_1 Y_{2_i} - k_2 Y_{3_i} Y_{8_i} Y_{6_i}^{\frac{1}{2}})$$

For Y_4

$$a_{1,4} = hf_4(t_i, \overline{Y_\iota})$$

$$a_{1,4} = h(2k_2 Y_{3_i} Y_{8_i} Y_{6_i}^{\frac{1}{2}} - 2k_4 Y_{4_i}^2)$$

For Y_5

$$a_{1,5} = hf_5(t_i, \overline{Y_\iota})$$

$$a_{1,5} = h(\frac{1}{2} k_2 Y_{3_i} Y_{8_i} Y_{6_i}^{\frac{1}{2}} + \frac{1}{2} k_3 Y_{7_i}^2 Y_{6_i}^{\frac{1}{2}} + 2k_4 Y_{4_i}^2)$$

For Y_6

$$a_{1,6} = hf_6(t_i, \overline{Y_\iota})$$

$$a_{1,6} = h(2k_1 Y_{2_i} - \frac{1}{2} k_2 Y_{3_i} Y_{8_i} Y_{6_i}^{\frac{1}{2}} - \frac{1}{2} k_3 Y_{7_i}^2 Y_{6_i}^{\frac{1}{2}} + 2k_4 Y_{4_i}^2)$$

For Y_7

$$a_{1,7} = hf_7(t_i, \overline{Y_\iota})$$

$$a_{1,7} = h(2k_1 Y_{2_i} - 2k_3 Y_{7_i}^2 Y_{6_i}^{\frac{1}{2}})$$

For Y_8

$$a_{1,8} = hf_8(t_i, \overline{Y_\iota})$$

$$a_{1,8} = h(-k_0 Y_{1_i} Y_{8_i} - k_2 Y_{3_i} Y_{8_i} Y_{6_i}^{\frac{1}{2}} + k_3 Y_{7_i}^2 Y_{6_i}^{\frac{1}{2}})$$

Value of a_2

For Y_1

$$a_{2,1} = hf_1(t_i + h, \overline{Y_\iota} + \overline{a_1})$$
$$a_{2,1} = h(-k_0(Y_{1_i} + a_{1,1})(Y_{8_i} + a_{1,8}))$$

For Y_2

$$a_{2,2} = hf_2(t_i + h, \overline{Y_\iota} + \overline{a_1})$$
$$a_{2,2} = h\left[k_0\left(Y_{1_i} + a_{1,1}\right)\left(Y_{8_i} + a_{1,8}\right) + k_1\left(Y_{2_i} + a_{1,2}\right)\right]$$

For Y_3

$$a_{2,3} = hf_3(t_i + h, \overline{Y_\iota} + \overline{a_1})$$
$$a_{2,3} = h\left[k_1\left(Y_{2_i} + a_{1,2}\right) - k_2\left(Y_{3_i} + a_{1,3}\right)\left(Y_{8_i} + a_{1,8}\right)\left(Y_{6_i} + a_{1,6}\right)^{\frac{1}{2}}\right]$$

For Y_4

$$a_{2,4} = hf_4(t_i + h, \overline{Y_i} + \overline{a_1})$$
$$a_{2,4} = h\left[2k_2\left(Y_{3_i} + a_{1,3}\right)\left(Y_{8_i} + a_{1,8}\right)\left(Y_{6_i} + a_{1,6}\right)^{\frac{1}{2}} - 2k_4\left(Y_{4_i} + a_{1,4}\right)^2\right]$$

For Y5

$$a_{2,5} = hf_5(t_i + h, \overline{Y_i} + \overline{a_1})$$
$$a_{2,5} = h[\tfrac{1}{2}k_2\left(Y_{3_i} + a_{1,3}\right)\left(Y_{8_i} + a_{1,8}\right)\left(Y_{6_i} + a_{1,6}\right)^{\frac{1}{2}} + \tfrac{1}{2}k_3\left(Y_{7_i} + a_{1,7}\right)^2\left(Y_{6_i} + a_{1,6}\right)^{\frac{1}{2}} + 2k_4\left(Y_{4_i} + a_{1,4}\right)^2]$$

For Y6

$$a_{2,6} = hf_6(t_i + h, \overline{Y_i} + \overline{a_1})$$
$$a_{2,6} = h[2k_1\left(Y_{2_i} + a_{1,2}\right) - \tfrac{1}{2}k_2\left(Y_{3_i} + a_{1,3}\right)\left(Y_{8_i} + a_{1,8}\right)\left(Y_{6_i} + a_{1,6}\right)^{\frac{1}{2}} - \tfrac{1}{2}k_3\left(Y_{7_i} + a_{1,7}\right)^2\left(Y_{6_i} + a_{1,6}\right)^{\frac{1}{2}} + 2k_4\left(Y_{4_i} + a_{1,4}\right)^2]$$

For Y7

$$a_{2,7} = hf_7(t_i + h, \overline{Y_i} + \overline{a_1})$$
$$a_{2,7} = h\left[2k_1\left(Y_{2_i} + a_{1,2}\right) - 2k_3\left(Y_{7_i} + a_{1,7}\right)^2\left(Y_{6_i} + a_{1,6}\right)^{\frac{1}{2}}\right]$$

For Y8

$$a_{2,8} = hf_8(t_i + h, \overline{Y_i} + \overline{a_1})$$
$$a_{2,8} = h[-k_0(Y_{1_i} + a_{1,1})(Y_{8_i} + a_{1,8}) - k_2\left(Y_{3_i} + a_{1,3}\right)\left(Y_{8_i} + a_{1,8}\right)\left(Y_{6_i} + a_{1,6}\right)^{\frac{1}{2}} + k_3\left(Y_{7_i} + a_{1,7}\right)^2\left(Y_{6_i} + a_{1,6}\right)^{\frac{1}{2}}]$$

- Fourth Order Runge-Kutta Method :
  For the kinetic system of ODE's given in Eq. (1), the RK method is modified to a vector equation to represent all the 8 ODE's as

$$\bar{Y}_{i+1} = \bar{Y}_i + \frac{1}{6}(\bar{a}_1 + 3\bar{a}_2 + 3\bar{a}_3 + \bar{a}_4) \tag{17}$$

where, $\bar{Y}_i = [\, Y_{1_i} \;\; Y_{2_i} \;\; \cdots \;\; Y_{8_i} \,]$

$\bar{a}_i = [\, a_{i,1} \;\; a_{i,2} \;\; \cdots \;\; a_{i,8} \,]$ for the given set of 8 ODE's.

For each application of the second order RK method, the values of $\underline{a}_1$, $\underline{a}_2, \underline{a}_3$ & $\underline{a}_4$ are calculated for each equation as follows

Value of a_1

For Y_1

$$a_{1,1} = hf_1(t_i, \overline{Y_i})$$
$$a_{1,1} = h(-k_0 Y_{1_i} Y_{8_i})$$

For Y_2

$$a_{1,2} = hf_2(t_i, \overline{Y_i})$$
$$a_{1,2} = h(k_0 Y_{1_i} Y_{8_i} + k_1 Y_{2_i})$$

For Y_3

$$a_{1,3} = hf_3(t_i, \overline{Y_i})$$
$$a_{1,3} = h(k_1 Y_{2_i} - k_2 Y_{3_i} Y_{8_i} Y_{6_i}^{\frac{1}{2}})$$

For Y_4

$$a_{1,4} = hf_4(t_i, \overline{Y_i})$$
$$a_{1,4} = h(2k_2 Y_{3_i} Y_{8_i} Y_{6_i}^{\frac{1}{2}} - 2k_4 Y_{4_i}^2)$$

For Y_5

$$a_{1,5} = hf_5(t_i, \overline{Y_i})$$
$$a_{1,5} = h(\tfrac{1}{2} k_2 Y_{3_i} Y_{8_i} Y_{6_i}^{\frac{1}{2}} + \tfrac{1}{2} k_3 Y_{7_i}^2 Y_{6_i}^{\frac{1}{2}} + 2k_4 Y_{4_i}^2)$$

For Y_6

$$a_{1,6} = hf_6(t_i, \overline{Y_i})$$
$$a_{1,6} = h(2k_1 Y_{2_i} - \tfrac{1}{2} k_2 Y_{3_i} Y_{8_i} Y_{6_i}^{\frac{1}{2}} - \tfrac{1}{2} k_3 Y_{7_i}^2 Y_{6_i}^{\frac{1}{2}} + 2k_4 Y_{4_i}^2)$$

For Y_7

$$a_{1,7} = hf_7(t_i, \overline{Y_i})$$
$$a_{1,7} = h(2k_1 Y_{2_i} - 2k_3 Y_{7_i}^2 Y_{6_i}^{\frac{1}{2}})$$

For Y_8

$$a_{1,8} = hf_8(t_i, \overline{Y_i})$$
$$a_{1,8} = h(-k_0 Y_{1_i} Y_{8_i} - k_2 Y_{3_i} Y_{8_i} Y_{6_i}^{\frac{1}{2}} + k_3 Y_{7_i}^2 Y_{6_i}^{\frac{1}{2}})$$

Value of a_2

For Y_1

$$a_{2,1} = hf_1\left(t_i + h, \overline{Y_i} + \frac{\overline{a_1}}{2}\right)$$

$$a_{2,1} = h(-k_0(Y_{1_i} + \frac{a_{1,1}}{2})(Y_{8_i} + \frac{a_{1,8}}{2}))$$

For Y_2

$$a_{2,2} = hf_2\left(t_i + h, \overline{Y_i} + \frac{\overline{a_1}}{2}\right)$$

$$a_{2,2} = h\left[k_0\left(Y_{1_i} + \frac{a_{1,1}}{2}\right)\left(Y_{8_i} + \frac{a_{1,8}}{2}\right) + k_1\left(Y_{2_i} + \frac{a_{1,2}}{2}\right)\right]$$

For Y_3

$$a_{2,3} = hf_3\left(t_i + h, \overline{Y_i} + \frac{\overline{a_1}}{2}\right)$$

$$a_{2,3} = h\left[k_1\left(Y_{2_i} + \frac{a_{1,2}}{2}\right) - k_2\left(Y_{3_i} + \frac{a_{1,3}}{2}\right)\left(Y_{8_i} + \frac{a_{1,8}}{2}\right)\left(Y_{6_i} + \frac{a_{1,6}}{2}\right)^{\frac{1}{2}}\right]$$

For Y_4

$$a_{2,4} = hf_4\left(t_i + h, \overline{Y_i} + \frac{\overline{a_1}}{2}\right)$$

$$a_{2,4} = h\left[2k_2\left(Y_{3_i} + \frac{a_{1,3}}{2}\right)\left(Y_{8_i} + \frac{a_{1,8}}{2}\right)\left(Y_{6_i} + \frac{a_{1,6}}{2}\right)^{\frac{1}{2}} - 2k_4\left(Y_{4_i} + \frac{a_{1,4}}{2}\right)^2\right]$$

For Y_5

$$a_{2,5} = hf_5\left(t_i + h, \overline{Y_i} + \frac{\overline{a_1}}{2}\right)$$

$$a_{2,5} = h[\tfrac{1}{2}k_2\left(Y_{3_i} + \frac{a_{1,3}}{2}\right)\left(Y_{8_i} + \frac{a_{1,8}}{2}\right)\left(Y_{6_i} + \frac{a_{1,6}}{2}\right)^{\frac{1}{2}} + \\ \tfrac{1}{2}k_3\left(Y_{7_i} + \frac{a_{1,7}}{2}\right)^2\left(Y_{6_i} + \frac{a_{1,6}}{2}\right)^{\frac{1}{2}} + 2k_4\left(Y_{4_i} + \frac{a_{1,4}}{2}\right)^2]$$

For Y_6

$$a_{2,6} = hf_6\left(t_i + h, \overline{Y_i} + \frac{\overline{a_1}}{2}\right)$$

$$a_{2,6} = h[2k_1\left(Y_{2_i} + \frac{a_{1,2}}{2}\right) - \tfrac{1}{2}k_2\left(Y_{3_i} + \frac{a_{1,3}}{2}\right)\left(Y_{8_i} + \frac{a_{1,8}}{2}\right)\left(Y_{6_i} + \frac{a_{1,6}}{2}\right)^{\frac{1}{2}} \\ -\tfrac{1}{2}k_3\left(Y_{7_i} + \frac{a_{1,7}}{2}\right)^2\left(Y_{6_i} + \frac{a_{1,6}}{2}\right)^{\frac{1}{2}} + 2k_4\left(Y_{4_i} + \frac{a_{1,4}}{2}\right)^2]$$

For Y_7

$$a_{2,7} = hf_7\left(t_i + h, \overline{Y_i} + \frac{\overline{a_1}}{2}\right)$$

$$a_{2,7} = h\left[2k_1\left(Y_{2_i} + \frac{a_{1,2}}{2}\right) - 2k_3\left(Y_{7_i} + \frac{a_{1,7}}{2}\right)^2\left(Y_{6_i} + \frac{a_{1,6}}{2}\right)^{\frac{1}{2}}\right]$$

For Y$_8$

$$a_{2,8} = hf_8\left(t_i + h, \overline{Y_i} + \frac{\overline{a_1}}{2}\right)$$

$$a_{2,8} = h[-k_0(Y_{1_i} + \frac{a_{1,1}}{2})(Y_{8_i} + \frac{a_{1,8}}{2}) -$$

$$k_2\left(Y_{3_i} + \frac{a_{1,3}}{2}\right)\left(Y_{8_i} + \frac{a_{1,8}}{2}\right)\left(Y_{6_i} + \frac{a_{1,6}}{2}\right)^{\frac{1}{2}} + k_3\left(Y_{7_i} + \frac{a_{1,7}}{2}\right)^2\left(Y_{6_i} + \frac{a_{1,6}}{2}\right)^{\frac{1}{2}}]$$

Value of a$_3$

For Y$_1$

$$a_{3,1} = hf_1\left(t_i + h, \overline{Y_i} + \frac{\overline{a_2}}{2}\right)$$

$$a_{3,1} = h(-k_0(Y_{1_i} + \frac{a_{2,1}}{2})(Y_{8_i} + \frac{a_{2,8}}{2}))$$

For Y$_2$

$$a_{3,2} = hf_2\left(t_i + h, \overline{Y_i} + \frac{\overline{a_2}}{2}\right)$$

$$a_{3,2} = h\left[k_0\left(Y_{1_i} + \frac{a_{2,1}}{2}\right)\left(Y_{8_i} + \frac{a_{2,8}}{2}\right) + k_1\left(Y_{2_i} + \frac{a_{2,2}}{2}\right)\right]$$

For Y$_3$

$$a_{3,3} = hf_3\left(t_i + h, \overline{Y_i} + \frac{\overline{a_2}}{2}\right)$$

$$a_{3,3} = h\left[k_1\left(Y_{2_i} + \frac{a_{2,2}}{2}\right) - k_2\left(Y_{3_i} + \frac{a_{2,3}}{2}\right)\left(Y_{8_i} + \frac{a_{,8}}{2}\right)\left(Y_{6_i} + \frac{a_{2,6}}{2}\right)^{\frac{1}{2}}\right]$$

For Y$_4$

$$a_{3,4} = hf_4\left(t_i + h, \overline{Y_i} + \frac{\overline{a_2}}{2}\right)$$

$$a_{3,4} = h\left[2k_2\left(Y_{3_i} + \frac{a_{2,3}}{2}\right)\left(Y_{8_i} + \frac{a_{2,8}}{2}\right)\left(Y_{6_i} + \frac{a_{2,6}}{2}\right)^{\frac{1}{2}} - 2k_4\left(Y_{4_i} + \frac{a_{2,4}}{2}\right)^2\right]$$

For Y$_5$

$$a_{3,5} = hf_5\left(t_i + h, \overline{Y_i} + \frac{\overline{a_2}}{2}\right)$$

$$a_{3,5} = h[\frac{1}{2}k_2\left(Y_{3_i} + \frac{a_{2,3}}{2}\right)\left(Y_{8_i} + \frac{a_{2,8}}{2}\right)\left(Y_{6_i} + \frac{a_{2,6}}{2}\right)^{\frac{1}{2}} +$$

$$\frac{1}{2}k_3\left(Y_{7_i} + \frac{a_{2,7}}{2}\right)^2\left(Y_{6_i} + \frac{a_{2,6}}{2}\right)^{\frac{1}{2}} + 2k_4\left(Y_{4_i} + \frac{a_{2,4}}{2}\right)^2]$$

For Y_6

$$a_{3,6} = hf_6\left(t_i + h, \overline{Y_i} + \frac{\overline{a_2}}{2}\right)$$

$$a_{3,6} = h[2k_1\left(Y_{2_i} + \frac{a_{2,2}}{2}\right) - \frac{1}{2}k_2\left(Y_{3_i} + \frac{a_{2,3}}{2}\right)\left(Y_{8_i} + \frac{a_{2,8}}{2}\right)\left(Y_{6_i} + \frac{a_{2,6}}{2}\right)^{\frac{1}{2}}$$
$$-\frac{1}{2}k_3\left(Y_{7_i} + \frac{a_{2,7}}{2}\right)^2\left(Y_{6_i} + \frac{a_{2,6}}{2}\right)^{\frac{1}{2}} + 2k_4\left(Y_{4_i} + \frac{a_{2,4}}{2}\right)^2]$$

For Y_7

$$a_{3,7} = hf_7\left(t_i + h, \overline{Y_i} + \frac{\overline{a_2}}{2}\right)$$

$$a_{3,7} = h\left[2k_1\left(Y_{2_i} + \frac{a_{2,2}}{2}\right) - 2k_3\left(Y_{7_i} + \frac{a_{2,7}}{2}\right)^2\left(Y_{6_i} + \frac{a_{2,6}}{2}\right)^{\frac{1}{2}}\right]$$

For Y_8

$$a_{3,8} = hf_8\left(t_i + h, \overline{Y_i} + \frac{\overline{a_2}}{2}\right)$$

$$a_{3,8} = h[-k_0(Y_{1_i} + \frac{a_{2,1}}{2})(Y_{8_i} + \frac{a_{2,8}}{2}) -$$
$$k_2\left(Y_{3_i} + \frac{a_{2,3}}{2}\right)\left(Y_{8_i} + \frac{a_{2,8}}{2}\right)\left(Y_{6_i} + \frac{a_{2,6}}{2}\right)^{\frac{1}{2}} + k_3\left(Y_{7_i} + \frac{a_{2,7}}{2}\right)^2\left(Y_{6_i} + \frac{a_{2,6}}{2}\right)^{\frac{1}{2}}]$$

Value of a_4

For Y_1

$$a_{4,1} = hf_1(t_i + h, \overline{Y_i} + \overline{a_3})$$

$$a_{4,1} = h(-k_0(Y_{1_i} + a_{1,1})(Y_{8_i} + a_{1,8}))$$

For Y_2

$$a_{4,2} = hf_2(t_i + h, \overline{Y_i} + \overline{a_3})$$

$$a_{4,2} = h\left[k_0\left(Y_{1_i} + a_{1,1}\right)\left(Y_{8_i} + a_{1,8}\right) + k_1\left(Y_{2_i} + a_{1,2}\right)\right]$$

For Y_3

$$a_{4,3} = hf_3(t_i + h, \overline{Y_i} + \overline{a_3})$$

$$a_{4,3} = h\left[k_1\left(Y_{2_i} + a_{1,2}\right) - k_2\left(Y_{3_i} + a_{1,3}\right)\left(Y_{8_i} + a_{1,8}\right)\left(Y_{6_i} + a_{1,6}\right)^{\frac{1}{2}}\right]$$

For Y_4

$$a_{4,4} = hf_4(t_i + h, \overline{Y_i} + \overline{a_3})$$

$$a_{4,4} = h\left[2k_2\left(Y_{3_i} + a_{1,3}\right)\left(Y_{8_i} + a_{1,8}\right)\left(Y_{6_i} + a_{1,6}\right)^{\frac{1}{2}} - 2k_4\left(Y_{4_i} + a_{1,4}\right)^2\right]$$

For Y_5

$$a_{4,5} = hf_5(t_i + h, \overline{Y_i} + \overline{a_3})$$

$$a_{4,5} = h[\tfrac{1}{2}k_2(Y_{3_i} + a_{1,3})(Y_{8_i} + a_{1,8})(Y_{6_i} + a_{1,6})^{\frac{1}{2}} + \tfrac{1}{2}k_3(Y_{7_i} + a_{1,7})^2(Y_{6_i} + a_{1,6})^{\frac{1}{2}} + 2k_4(Y_{4_i} + a_{1,4})^2]$$

For Y6

$$a_{4,6} = hf_6(t_i + h, \overline{Y_i} + \overline{a_3})$$

$$a_{4,6} = h[2k_1(Y_{2_i} + a_{1,2}) - \tfrac{1}{2}k_2(Y_{3_i} + a_{1,3})(Y_{8_i} + a_{1,8})(Y_{6_i} + a_{1,6})^{\frac{1}{2}} - \tfrac{1}{2}k_3(Y_{7_i} + a_{1,7})^2(Y_{6_i} + a_{1,6})^{\frac{1}{2}} + 2k_4(Y_{4_i} + a_{1,4})^2]$$

For Y7

$$a_{4,7} = hf_7(t_i + h, \overline{Y_i} + \overline{a_3})$$

$$a_{4,7} = h\left[2k_1(Y_{2_i} + a_{1,2}) - 2k_3(Y_{7_i} + a_{1,7})^2(Y_{6_i} + a_{1,6})^{\frac{1}{2}}\right]$$

For Y8

$$a_{4,8} = hf_8(t_i + h, \overline{Y_i} + \overline{a_3})$$

$$a_{4,8} = h[-k_0(Y_{1_i} + a_{1,1})(Y_{8_i} + a_{1,8}) - k_2(Y_{3_i} + a_{1,3})(Y_{8_i} + a_{1,8})(Y_{6_i} + a_{1,6})^{\frac{1}{2}} + k_3(Y_{7_i} + a_{1,7})^2(Y_{6_i} + a_{1,6})^{\frac{1}{2}}]$$

3.4 By Younker's Modified Adomian Decomposition Method

(In the text, i varies from 1 to 8)

As we have found out that ADM is a semi-analytical method, which uses a lot of terms to compute the answer, making program space as well as time inefficient. So J.M. Younker proposed a modification to ADM, so that it can be used to find solutions of differential equations.

Splitting into Time Dependent and Time Independent Parts

Time dependent concentrations make it harder to integrate the function. So, in this modification, time dependent and time independent parts are separated and solved separately.

In general,

$$y_k = y_k(0) + L^{-1}[R_k(t, y_1, y_2, \dots, y_m) + N_k(t, y_1, y_2, \dots, y_m)] \qquad (18)$$

Instead of using y_k, we use $\vec{y}$ to represent solution, such that

$$\vec{y} = \vec{y}(0) + \hat{Y}\vec{b}(t) \tag{19}$$

where, $\vec{y}(0)$ represents the initial concentration, $\hat{Y}$ represents the time independent and $\vec{b}(t)$ represents the time dependent term, such that $\hat{Y}\vec{b}(t)$ is the vector form of second term on RHS of equation (18).

Solving for $\hat{Y}_{i,j}$

- $\hat{Y}_{(i,0)}$

  Using ADM, we can write:

$$\begin{aligned} y_{(i,1)}(t) &= L^{-1}(t)\left[A_{(i,0)}\big(\vec{y}(t)\big) + \textstyle\sum_{j=1}^{p} k_{(i,j)} y_{(j,0)}(t)\right] \\ &= L^{-1}(t)\left[f_i\big(\vec{y}(0)\big)\right] \\ &= t\left[f_i\big(\vec{y}(0)\big)\right] && (20) \\ &= t\hat{Y}_{(i,0)} && (21) \end{aligned}$$

- $\hat{Y}_{(i,1)}$

$$\begin{aligned} y_{(i,2)}(t) &= L^{-1}(t)\left[A_{(i,1)}\big(\vec{y}(t)\big) + \sum_{j=1}^{p} k_{(i,j)} y_{(j,1)}(t)\right] \\ &= L^{-1}(t)\left[t\sum_{j=1}^{p}(\hat{Y}_{(j,0)} + \frac{\partial f_i\big(\vec{y}(0)\big)}{\partial y_j})\right] \\ &= \frac{t^2}{2!}\left[\textstyle\sum_{(j=0)}^{p} \hat{Y}_{(i,0)} \frac{\partial f_i \vec{y}(0)}{\partial y_j}\right] && (22) \\ &= \frac{t^2}{2!}(\hat{Y}_{(i,1)}) && (23) \end{aligned}$$

Time Dependent Part

The time dependent part, $b_n(t)$, is separated from time independent part to simplify computations. In $b_n(t)$, n = j+1, where j is the second index of $\hat{Y}$. (Like for $\hat{Y}_{(1,0)}, n = 0 + 1 = 1$)

General expression: $$b_n(t) = \frac{t^{n+1}}{(n+1)!} \tag{24}$$

Finally, let y_i stores the i^{th} component of solution vector, $\vec{y}$. Then y_i is given by:

$$y_i = y_i(0) + \sum_{n=0}^{n_{Max}} \frac{t^{n+1}}{(n+1)!} \hat{Y}_{(i,n)} \tag{25}$$

Where $n_{Max} = 1$ in our case. So, the final expression for solution is:

$$y_i = y_i(0) + t\hat{Y}_{(i,0)} + \frac{t^2}{2!} \hat{Y}_{(i,1)} \tag{26}$$

4. Results and Discussion:

- **Runge-Kutta Methods:** The set of kinetic system of ODE's in Eq. (1) is solved by these two Runge-Kutta Methods by solving the above equations to find a_i's in each iteration to find the next Y_{i+1} data point at $t_{i+1} = t_i + h$.
  The simulation is performed considering a step size of h = 0.1 days and considering the concentrations of the starting materials Cellulose (Y_1) & Water (Y_8) to be 1 mol/L.
  Figure 1 shows the results obtained for Cellulose concentrations and the product Biogas against time for the second-order Runge-Kutta Method, while Figure 2 shows the results for the fourth-order Runge-Kutta Method.

  The anaerobic decomposition of glucose, obtained as a product from cellulose at 100% substrate, as a whole is given as $C_6H_{12}O_6 \rightarrow 3CH_4 + 3CO_2$. Starting with 1 mole of 100% glucose, 6 moles of biogas can be obtained theoretically. The results obtained from the RK methods are consistent with this fact, and have successfully replicated the data presented in the original paper.

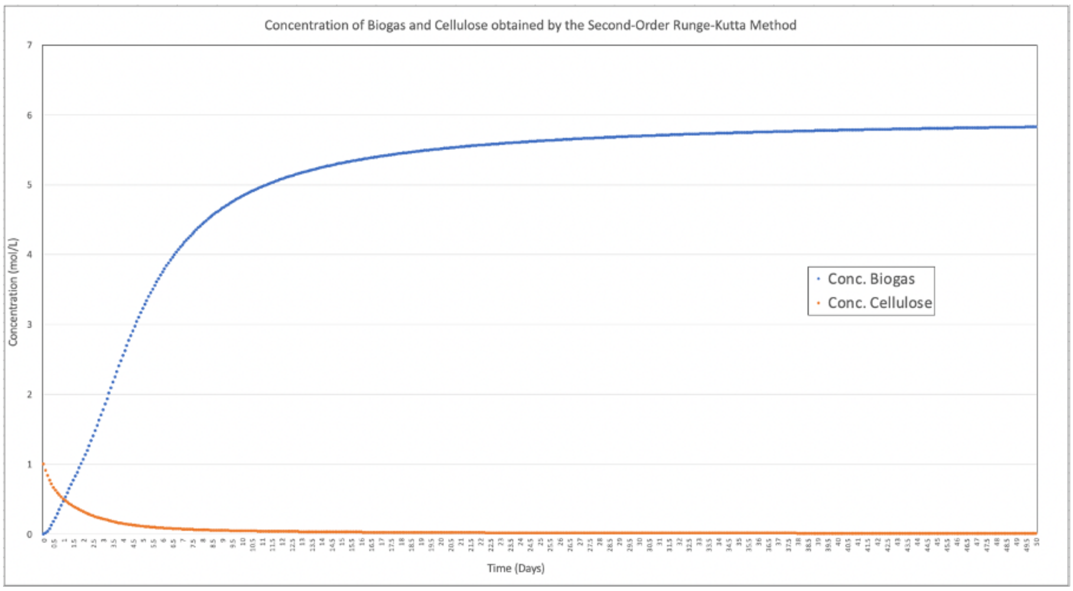

Figure 1: Concentration of Biogas and Cellulose obtained by the second-order RK Method

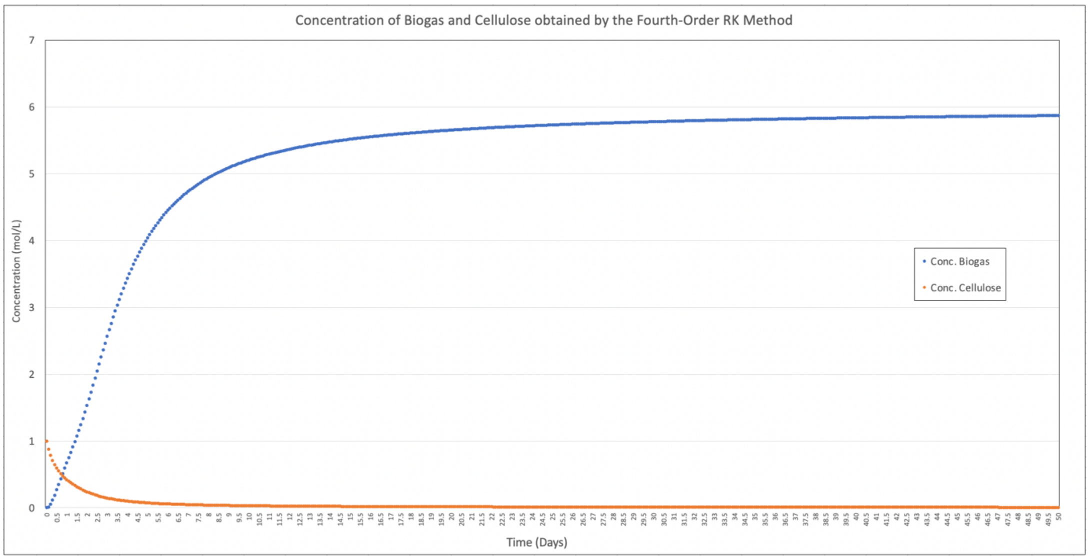

Figure 2: Concentration of Biogas and Cellulose obtained by the fourth-order RK Method

- **ADM:** ADM is a semi analytical method, so we need to include many terms to get an accurate answer. Clearly in our code, we can’t include a lot of terms as it makes the program time and space inefficient. Due to this, the code doesn’t converge to the concentration obtained from the RK-2/ RK-4 method. Even in the original paper, ADM couldn’t obtain output, so Modified ADM had to be used.

- **Modified ADM:** When we use the modification mentioned in part (3.4) in our code, we find that the solution converges very quickly to the concentration of biogas (in almost 3 days), which is inconsistent with the results obtained from RK-2 and RK-4 methods as well as the data given in the original paper.
  The problem arises because of the following reasons:
  - limited number of terms $(n_{Max} = 1)$. We can get a better solution for the problem if we extend n_{Max} to higher values 3 or 4.
  - presence of 2nd and higher order partial derivatives, which is out of the scope of course, makes it difficult to compute $\widehat{Y}_{(i,2)}, \widehat{Y}_{(i,3)}$ and other higher order terms.
  - updating the values of 'f' after every single iteration, instead of updating after a time of, say 1 day.

  The diverging output can be seen in the output files enclosed.

5. Conclusion:

Based on the above results, we made the following conclusions:

- In the process of generation of Biogas from biomass, the major conversion takes place in the first 10 days after the start of the process, and the process slows down drastically after 25-30 days.
- Second-order & fourth-order Runge-Kutta methods are simple yet effective in solving a kinetic system of ODEs.
- While solving a system of differential equations with a single independent variable, the modified Adomian Decomposition Method computes the concentrations of different species as a function of that independent variable.
- The Modified Adomian Decomposition Method is more space and time efficient than the classical ADM.
- Computational application of ADM/MADM was significantly more challenging than the RK methods owing to lack of prior knowledge and understanding.

6. Self-Assessment:

In this paper, we managed to develop a chemical and mathematical model of the Anaerobic Digestion process using second-order Runge-Kutta Method and proceeded to utilize the modified version of a new method called Adomian Decomposition to replicate the results.

We developed C++ programs to solve non-linear and coupled ordinary differential equations generated in our chosen process. We were able to obtain exact results by RK-2 method and faced some computational problems in the code for the Adomian method. We have attached our codes and some graphs for reference.

We wished to experiment further with RK methods since we were more familiar with it due to this course. So we developed a code for a fourth-order RK method to solve the same problem as well and utilized it to compare our results from RK-2.

Our main objective was to obtain results from the RK-2 method and compare them with the approach of ADM. Our extension in the paper was to include a higher order of RK method to see if our results could be optimized. We plotted the results obtained from the three codes and compared it with the analytical solution and the result was quite similar, as can be seen in the graphs.

We learned concepts of Anaerobic Digestion and ways to apply the numerical methods taught in class to solve the kinetic system of equations. We also received exposure to a new method and the research done to utilize it in the paper has improved our understanding of it. We have thus learned to apply concepts of numerical methods to real chemical engineering problems.

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