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Comparison of the Modified Adomian Decomposition Method and the Simplified Runge-Kutta Method for Solutions of the Anaerobic Digestion Process

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Abstract. The model that describes the transformation of biomass into biogas, a process called Anaerobic Digestion, is complex because it involves nonlinear and coupled ordinary differential equations. In this way, obtaining an analytical-numerical solution becomes attractive for this problem. In this paper, the chemical kinetics of the anaerobic digestion process is modelade. The system of equations of the model was solved by the Modified Adomian Decomposition Method, a powerful technique used for solve systems of linear and nonlinear differential equations, since it is computationally convenient, precise and physically realistic. The results are compared with the data obtained by the second-order Simplified Runge-Kutta method, and they agree well with each other.

Keywords. Anaerobic digestion, Biogas, Simplified Runge-Kutta, Adomian decomposition method

1 Introduction

Anaerobic digestion (AD) is a biochemical biogas production process. Biogas is a biofuel composed mainly by methane and carbon dioxide [16]. In this process, biofuel is formed from the biological degradation of biomass [15], the world's most abundant raw material consisting of substances of organic origin, such as plant, animal and microorganisms.

Anaerobic digestion is a complex process, consisting of several stages of metabolic interactions, in the absence of oxygen, and performed by a well-organized community of microbial populations [5,11]. The mathematical model is obtained according to the number of chemical reactions presented in each stage of the process. This modeling provides a set of coupled and nonlinear ordinary differential equations.

The Adomian Decomposition Method (ADM) is a powerful technique used to solve this problem, which involves the writing of nonlinear terms in a series of polynomials.

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Adomian [2] demonstrated that with the ADM technique it is possible solve linear and nonlinear differential equations, obtaining continuous solutions.

Currently, the ADM technique has been used by many authors in several areas to solve problems of linear and nonlinear equations, involving initial and/or boundary conditions [3, 9, 10]. In addition, this technique can be used to solve systems of nonlinear differential equations and also to the solution of higher-order differential equations [4, 8]. Some researchers have introduced modifications in the ADM technique [1, 7]. For example, Younker [14] modified the ADM to solve a system of coupled differential equations describing chemical reaction rates.

In this work, 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 by the Modified Adomian Decomposition, applied to the time variable [14], and Simplified Runge-Kutta [6] methods. The two approximations to the solution are compared and one concludes that they agree well.

2 Chemical and mathematical modeling

The phases and reactions of the anaerobic digestion process are:

(I) Hydrolysis:

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

(II) Acidogenesis:

$$C_6H_{12}O_6 \rightarrow C_4H_8O_2 + 2CO_2 + 2H_2, \quad \Delta\text{G} = -264,19 \text{ KJ/mol}.$$

(III) Acetogenesis:

$$2C_4H_8O_2 + 2H_2O + CO_2 \rightarrow 4C_2H_4O_2 + CH_4, \quad \Delta\text{G} = -35 \text{ KJ/mol}.$$

(IV) Hydrogenotrophic methanogenesis:

$$4H_2 + CO_2 \rightarrow CH_4 + 2H_2O, \quad \Delta\text{G} = -131 \text{ KJ/mol}.$$

(V) Acetoclastic methanogenesis:

$$C_2H_4O_2 \rightarrow CH_4 + CO_2, \quad \Delta\text{G} = -36 \text{ KJ/mol}.$$

More details on each phase can be found in [12].

Table 1 shows the chemical compounds involved in the anaerobic digestion process, described above. Each chemical compound is associated with its chemical formula and abbreviations.

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Tabela 1: Chemical compounds, chemical formulas and abbreviations.

Chemical compounds	**Chemical formulas**	**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
Hidrogen	H_2	Y_7
Water	H_2O	Y_8

The mathematical formulation of the anaerobic digestion process is associated to the phases described above: (I), (II), (III), (IV), and (V). The mathematical model provides a set of ordinary differential equations, called *kinetic system of ordinary differential equations* (ODEs) (see [13]).

The kinetic system of ODEs and its initial values provides the following initial value problem:

$$\left\{\begin{array}{ll}
\dfrac{dY_1}{dt} = -k_0Y_1Y_8, & Y_1(0) = 1 \\
\dfrac{dY_2}{dt} = k_0Y_1Y_8 - k_1Y_2, & Y_2(0) = 0 \\
\dfrac{dY_3}{dt} = k_1Y_2 - k_2Y_3Y_8Y_6^{1/2}, & Y_3(0) = 0 \\
\dfrac{dY_4}{dt} = 2k_2Y_3Y_8Y_6^{1/2} - 2k_4Y_4^2, & Y_4(0) = 0 \\
\dfrac{dY_5}{dt} = \dfrac{1}{2}k_2Y_3Y_8Y_6^{1/2} + \dfrac{1}{2}k_3Y_6^{1/2}Y_7^2 + 2k_4Y_4^2, & Y_5(0) = 0 \\
\dfrac{dY_6}{dt} = 2k_1Y_2 - \dfrac{1}{2}k_2Y_3Y_8Y_6^{1/2} - \dfrac{1}{2}k_3Y_6^{1/2}Y_7^2 + 2k_4Y_4^2, & Y_6(0) = 0 \\
\dfrac{dY_7}{dt} = 2k_1Y_2 - 2k_3Y_6^{1/2}Y_7^2, & Y_7(0) = 0 \\
\dfrac{dY_8}{dt} = -k_0Y_1Y_8 - k_2Y_3Y_8Y_6^{1/2} + k_3Y_6^{1/2}Y_7^2, & Y_8(0) = 1
\end{array}\right. . \tag{1}$$

3 Solution of the problem

The system (1)are solved by two methods:

1) Modified Adomian Decomposition (Modified ADM)

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The solution is obtained with a truncated series of Adomian polynomials, using the Adomian decomposition method, applied to the time variable [14].

2) Second-order Simplified Runge-Kutta method (RKsimp)
This method provides a good approximation for the solution of systems of coupled equations and is characterized by the small number of operations performed [6].

4 Results and discussion

Assume that $k_0 = 1$ and the constants k_1, k_2, k_3 and k_4 are estimated using the Gibbs free energy value (ΔG^o) (see [13]).

The simulation is performed using the Modified Adomian and Simplified Runge-Kutta methods, considering $h = 0.1$. Figure 1 (a) shows the solution obtained for biogas production. It is shown that biogas production increases rapidly in the first days of the process. After that, the solution slowly tends to the value six, indicating that the methanogenic phase continues for about 50 days. Figure 1 (b) show the errors

$$E_\infty^B = \max |Y_B - \tilde{Y}_B|,$$

where Y_B and $\tilde{Y}_B$ are the biogas concentrations vector using Modified ADM and RKsimp, respectively.

The errors are calculated for different values of h (for different numbers of mesh points). The objective is to compare the two solutions by calculating the difference between them when the number of points of the mesh increases. It is observed that the errors decrease as the spacing between the points decreases, showing that there is agreement between the two solutions.

5 Conclusions

In this work, we developed a model for the biogas production process, considering cellulose as substrate. With the Gibbs free energy value (ΔG), the production rate of each reaction is estimated.

The anaerobic decomposition of glucose, as a cellulose product at 100% substrate, is possibly given as a whole by $C_6H_{12}O_6 = 3CH_4 + 3CO_2$, i.e, with 1 kmol of 100% glucose, 6 kmol of biogas can be produced, which is consistent with the results obtained. This shows that, with a computationally simple model, we can solve the coupled set of nonlinear ordinary differential equations, obtained from the anaerobic digestion problem.

In addition, the Modified ADM solution, used for comparison with numerical results, is an important contribution of the present study.

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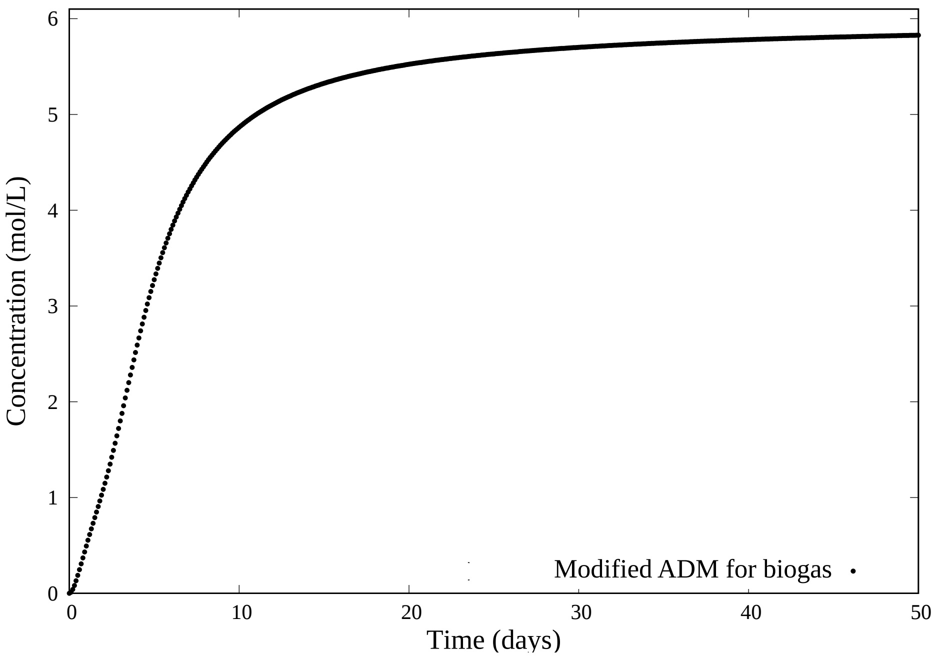
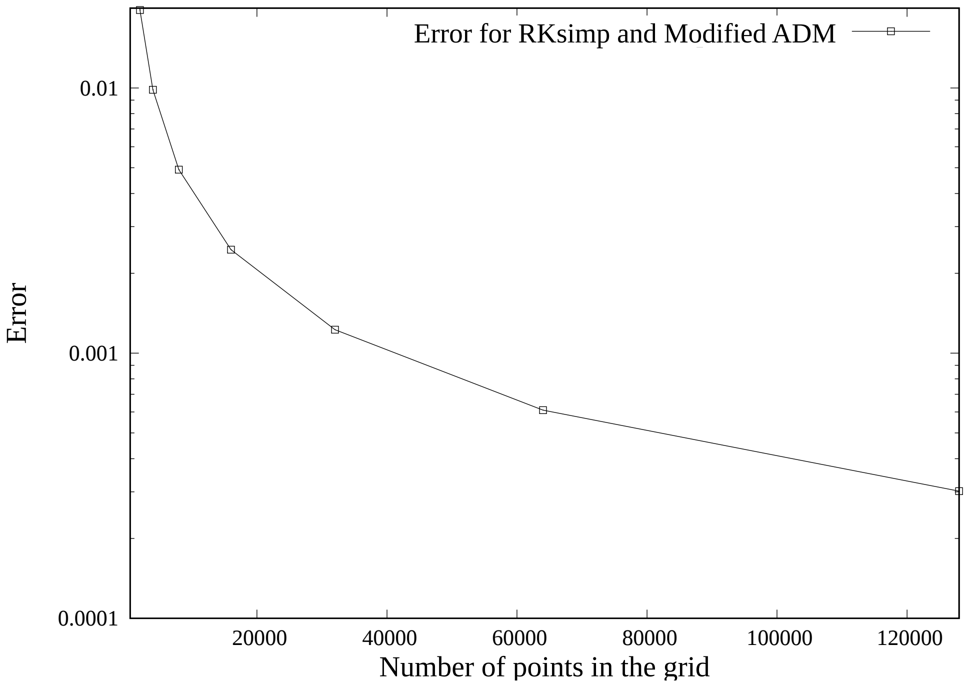


(a) Concentration of biogas obtained by the Modified ADM.



(b) Difference between Modified ADM and RKsimp.

Figura 1: Simulations for the biogas production process.

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