

THE FRANK'S KINETIC MODEL THROUGH THE ADOMIAN'S DECOMPOSITION METHOD

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Abstract: In this work we consider the Frank kinetic model [7] recently studied by Gutman [10] in a framework where the resources are limited. The model consists of a nonlinear system of differential equations for which we propose an alternative solution through the Adomian decomposition method (ADM).

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1. Introduction

Most of the dynamic phenomena arising in nature are described by nonlinear differential equations (ordinary or partial) and in some cases by integral equations. However, most of the methods developed in mathematics are used to solve linear differential equations. In general, the decomposition method developed by the mathematician George Adomian (1923-1996), has been very useful in applied mathematics [12], [13]. The Adomian decomposition method (ADM) has the advantage that it converges to the exact solution in a vast majority of very important cases in applications and can be handled easily for a wide class

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of differential equations (ordinary and partial) both linear and nonlinear systems of differential equations. In this paper we will use the ADM to specifically solve the system of nonlinear differential equations resulting from the kinetic Frank model [7] that has been extensively studied and analyzed by Gutman in [10] and [8].

2. The Frank Kinetic Model

All living organisms contain (optically active) chiral molecules and only a series of enantiomers is present. Specifically, biochemical processes in all living organisms involve *L*-amino acids and *D*-sugars; with a total absence of their counterparts (in a mirror image), that is, *D*-amino acids and *L*-Sugars. Furthermore, when living organisms and their products (particularly enzymes) are excluded, then chiral substances are formed as racemic mixtures containing equal amounts of both enantiomeric forms; this stereochemical difference between living and nonliving matter has puzzled scientists since the time of Louis Pasteur [11].

In 1953, Frank [7] proposed a model using the law of mass action that consists of the following chemical reactions:



In (1) a pair of enantiomers *R* and *S* are produced in an autocatalytic process in which *A* is an achiral reactant. Enantiomers *R* and *S* are eliminated each other resulting in an inactive product:



Mathematically, assuming that enantiomers are time-dependent $R = R(t)$, $S = S(t)$ and the achiral reactant *A* as a constant *a*, we have that the Frank model is expressed in the following system of nonlinear differential equations:

$$\begin{aligned} \frac{dR}{dt} &= k_1 a R - k_2 R S, \\ \frac{dS}{dt} &= k_1 a S - k_2 R S. \end{aligned} \tag{3}$$

3. Adomian Decomposition Method

The ADM method allows to find an analytical solution for an ordinary differential equation or an equation in partial derivatives, [4]. The method consists of identifying in the differential equation, the linear and the nonlinear parts, then inverting the differential operator of higher order of the linear part, and considering the unknown function as a series whose terms will be determined through ADM; in the next step, the nonlinear part is decomposed in terms of Adomian polynomials, [3]. We define the initial and/or boundary conditions and the terms involving the independent variable as the first approach. Thus, the unknown terms of the series can be found through recursive relationships.

In general, the method is the following: given a differential equation (ordinary or partial)

$$Fu(x, t) = g(x, t) \quad (4)$$

with initial condition

$$u(x, 0) = f(x), \quad (5)$$

where F represents a linear combination of differential operators involving both the linear, nonlinear terms and then equation (4) can be written as

$$L_t u(x, t) + Ru(x, t) + Nu(x, t) = g(x, t), \quad (6)$$

where $L_t = \frac{\partial}{\partial t}$, R is a linear operator involving derivatives (ordinary or partial) with respect to x and N is a nonlinear operator; g is a non-homogeneous term independent of u .

From equation (6), we have

$$L_t u(x, t) = g(x, t) - Ru(x, t) - Nu(x, t). \quad (7)$$

Since L is invertible, acting on (7) with the inverse $L_t^{-1}(\cdot) = \int_0^t (\cdot) ds$, we obtain

$$L_t^{-1} L_t u(x, t) = L_t^{-1} g(x, t) - L_t^{-1} Ru(x, t) - L_t^{-1} Nu(x, t) \quad (8)$$

and thus, an equivalent expression to equation (8) is

$$u(x, t) = f(x) + L_t^{-1} g(x, t) - L_t^{-1} Ru(x, t) - L_t^{-1} Nu(x, t), \quad (9)$$

where $f(x)$ is the constant of integration (with respect to t) such that $L_t f = 0$. The ADM method [4], decomposes the solution of (4), (5) into a series given by

$$u(x, t) = \sum_{n=0}^{\infty} u_n(x, t). \quad (10)$$

The non-linear term $Nu(x, t)$ decomposes in turn as

$$Nu(x, t) = \sum_{n=0}^{\infty} A_n(u_0, u_1, \dots, u_n), \quad (11)$$

where $\{A_n\}_{n=0}^{\infty}$, is the so called Adomian polynomials sequence see, e.g [1] and [2].

Replacing now equations (10), (11) into (9), we find

$$\sum_{n=0}^{\infty} u_n(x, t) = f(x) + L_t^{-1}g(x, t) - L_t^{-1}R \sum_{n=0}^{\infty} u_n(x, t) - L_t^{-1} \sum_{n=0}^{\infty} A_n, \quad (12)$$

from where the recursive algorithm can be obtained, for every $n = 0, 1, 2, \dots$

$$\begin{cases} u_0(x, t) = f(x) + L_t^{-1}g(x, t), \\ u_{n+1}(x, t) = L_t^{-1}Ru_n(x, t) - L_t^{-1}A_n(u_0, u_1, \dots, u_n). \end{cases} \quad (13)$$

With the algorithm (13) we can obtain an approximate solution of (4), (5) through the series

$$u(x, t) \approx \sum_{n=0}^k u_n(x, t), \quad \text{with} \quad \lim_{k \rightarrow \infty} \sum_{n=0}^k u_n(x, t) = u(x, t). \quad (14)$$

The series decomposition of the solution usually converges faster. Because of this, only a few terms are required to analyze. The conditions for which the method converges have been studied in the work [5], [6], [1] and mainly [2]. In the case of systems of differential equations, each of the dependent variables are recursively obtained with (13) and the approach to the solutions in each case with (14).

In the next section we consider the ADM to decompose a system of nonlinear ordinary differential equations and propose an example to compare the goodness of the method with the exact solution.

4. Decomposition of the Frank's Model

To solve the system (3) with A a constant through the ADM method, we assume that $k_1a = a_1 \neq 0$ and $k_2 = a_2 \neq 0$ and thus (3) can be rewritten as

$$\begin{aligned} \frac{dR}{dt} &= a_1R - a_2RS, \\ \frac{dS}{dt} &= a_1S - a_2RS, \end{aligned} \quad (15)$$

then defining $\tau = a_1 t$, $u(\tau) = \frac{a_1}{a_2} R(t)$, $v(\tau) = \frac{a_2}{a_1} S(t)$, $\beta = \frac{a_2^2}{a_1^2}$, the system of equations (15) becomes the non-linear system of differential equations

$$\begin{aligned}\frac{du}{d\tau} &= u - uv \\ \frac{dv}{d\tau} &= v - \beta uv\end{aligned}\tag{16}$$

with initial conditions $u(0) = u_0$, $v(0) = v_0$. To find the solutions u and v satisfying (16), we use the ADM to obtain

$$u(\tau) = \sum_{n=0}^{\infty} u_n(\tau), \quad v(\tau) = \sum_{n=0}^{\infty} v_n(\tau),\tag{17}$$

where, according to (13), if $n \geq 0$ we find the recursive solution

$$u_{n+1}(\tau) = \int_0^\tau (u_n - A_{1,2,n}) ds, \quad v_{n+1}(\tau) = \int_0^\tau (v_n - \beta A_{2,1,n}) ds,\tag{18}$$

and

$$A_{1,2,n} = \sum_{k=0}^n u_k v_{n-k}, \quad A_{2,1,n} = \sum_{k=0}^n v_k u_{n-k}.\tag{19}$$

Example 1. As an example of using the ADM method through (18) and (19) consider $k_1 = 1/2$, $k_2 = 1$, $a = 2$ and thus $\beta = 1$ in (3) as well as the initial conditions $u_0 = 2$ and $v_0 = 1$ ($u_0 > v_0$). With these data we have:

$$(\text{for } n = 0) \quad \begin{cases} A_{1,2,0}(t) = 2 \\ A_{2,1,0}(t) = 2 \\ u_1(t) = 0 \\ v_1(t) = -t \end{cases}\tag{20}$$

$$(\text{for } n = 1) \quad \begin{cases} A_{1,2,1}(t) = 2 \\ A_{2,1,1}(t) = 1 - 2t \\ u_2(t) = -2t \\ v_2(t) = \frac{t^2}{2} - t \end{cases}\tag{21}$$

$$(\text{for } n = 2) \quad \begin{cases} A_{1,2,2}(t) = t^2 - 4t \\ A_{2,1,2}(t) = t^2 - 4t \\ u_3(t) = -\frac{1}{3}t^3 + t^2 \\ v_3(t) = -\frac{1}{6}t^3 + \frac{3}{2}t^2 \end{cases}\tag{22}$$

$$(\text{for } n = 3) \quad \begin{cases} A_{1,2,3}(t) = -\frac{2}{3}t^3 + 4t^2 - 2t \\ A_{2,1,3}(t) = -\frac{2}{3}t^3 + 6t^2 \\ u_4(t) = \frac{1}{12}t^4 - t^3 + t^2 \\ v_4(t) = \frac{1}{8}t^4 - \frac{3}{2}t^3 \end{cases} \quad (23)$$

$$(\text{for } n = 4) \quad \begin{cases} A_{1,2,4}(t) = -\frac{2}{3}t^3 + 4t^2 - 2t \\ A_{2,1,4}(t) = -\frac{2}{3}t^3 + 6t^2 \\ u_5(t) = -\frac{7}{60}t^5 + \frac{5}{4}t^4 - \frac{2}{3}t^3 \\ v_5(t) = -\frac{13}{120}t^5 + \frac{7}{8}t^4 - \frac{2}{3}t^3 \end{cases} \quad (24)$$

$$\vdots$$

With these we can do the approach to fifth order as $\tau = a_1 t = k_1 a t = t$, and get

$$u(t) \approx 2 - 2t + 2t^2 - 2t^3 + \frac{4}{3}t^4 - \frac{7}{60}t^5, \quad (25)$$

$$v(t) \approx 1 - 2t + 2t^2 - \frac{7}{3}t^3 + t^4 - \frac{13}{120}t^5. \quad (26)$$

In Table 1 we show the results obtained with the ADM method and comparing with those exact values of $r(t)$ and $s(t)$ for (3) obtained in [10], that, considering a as a constant are given by

$$r(t) = r_0(r_0 - s_0)(r_0 - s_0 F)^{-1} e^{k_1 a t},$$

$$s(t) = s_0(r_0 - s_0)F(r_0 - s_0 F)^{-1} e^{k_1 a t},$$

where F , after a small correction relative to its value obtained in [10], is given by

$$F(t) = \exp \left(-\frac{k_2}{k_1 a} (r_0 - s_0) [e^{k_1 a t} - 1] \right).$$

As we see from Table 1, the absolute difference between these variables is about 2×10^{-5} .

time t	$u(t)$	$v(t)$	$r(t)$ exact	$s(t)$ exact
0.0	2.00000	1.00000	2.00000	1.00000
0.1	1.81813	0.81776	1.81815	0.81778
0.2	1.66617	0.66289	1.66619	0.66291
0.3	1.53652	0.52483	1.53654	0.52485
0.4	1.42494	0.48568	1.42496	0.48570
0.5	1.32969	0.44434	1.32971	0.44436
0.6	1.25173	0.40329	1.25175	0.40330
0.7	1.19453	0.39515	1.19455	0.39517
0.8	1.16399	0.26744	1.16401	0.26746
0.9	1.16791	0.13717	1.16793	0.13719
1.0	1.21667	0.00155	1.21669	0.00157

Table 1: The exact values [10] and the ADM values in $t \in [0, 1]$.

5. Summary

In this work the Adomian decomposition method has been implemented to solve the version of the Frank kinetic model in which the amount of achiral reactant A remains constant. The approximation by Adomian polynomials of fifth degree, gives an approximation of the amount of enantiomers with an error of order 2×10^{-5} . Moreover, in Table 1 we compare with the results of [9] concerning the enantiomeric excess of ee when $t \rightarrow \infty$. Our approach is consistent since with A constant $ee \rightarrow 1$ when $t \rightarrow \infty$.

We have used the *Mathematica* package has been used to calculate the decomposition series.

References

- [1] K. Abbaoui, Y. Cherruault, Convergence of Adomian's method applied to differential equations, *Computers and Mathematics with Applications*, **28** (1994), 103-109.
- [2] K. Abbaoui, Y. Cherruault, New ideas for proving convergence of decomposition methods, *Computers and Mathematics with Applications*, **29** (1995), 103-108.
- [3] G. Adomian, A review of the decomposition method in applied mathe-

- matics, *Journal of Mathematical Analysis and Applications*, **135** (1988), 501-544.
- [4] G. Adomian, *Solving Frontier Problems of Physics: The Decomposition Method*, Kluwer Academic Publishers, Boston, MA (1994).
- [5] Y. Cherruault, Convergence of Adomian's method, *Kybernetes*, **18** (1989), 31-38.
- [6] Y. Cherruault, G. Adomian, Decomposition methods: a new proof of convergence, *Mathematical and Computer Modelling*, **18** (1993), 103-106.
- [7] F.C. Frank, On spontaneous asymmetric synthesis, *Biochimica et Biophysica Acta*, **11** (1953), 459-463.
- [8] I. Gutman, Factors determining the direction of the stereoselection process in the generalized Frank model, *Journal of Mathematical Chemistry*, **3** (1989), 343-355.
- [9] I. Gutman, The Frank kinetic model for spontaneous chiral symmetry breaking with variable concentration of the achiral substrate, *Journal of Science Islamic Republic of Iran*, **6** (1995), 231-234.
- [10] I. Gutman, Frank model with limited resources, *Journal of Mathematical Chemistry*, **52** (2014), 2330-2333.
- [11] L. Pasteur, *Sur la dissymétrie moléculaire*, In: *Leçons de chimie professées en 1860 par M.M. Pasteur*, Cahours, Wurtz, Berthelot, Sante-claire Deville, Barral, et Dumas, Hachette, Paris (1881).
- [12] M. Tatari, M. Dehghan, The use of the Adomian decomposition method for solving multipoint boundary value problems, *Physica Scripta*, **73** (2006), 672-676.
- [13] A.M. Wazwaz, *Partial Differential Equations: Methods and Applications*, Balkema Publishers, Lisse, Netherlands (2002).