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Solving the Chemical Reaction Models with the Upadhyaya Transform

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ABSTRACT

In this article, the Upadhyaya transform is employed in diverse chemical reaction models expressed through ordinary differential equations. The investigation reveals that this transform provides precise and efficient solutions, circumventing the necessity for complex computations. Furthermore, the integration of graphical representations enhanced the interpretability of results, offering visual insights into the temporal evolution of reactant concentrations. These findings collectively underscore the efficacy of the Upadhyaya transform in addressing ordinary differential equations within chemical reaction models.

Keywords: Upadhyaya transform, Inverse Upadhyaya transform, Chemical reaction model, Ordinary differential equation.

INTRODUCTION

Differential equations have frequently been solved using the integral transform. Due to their significance in mathematically expressing potential changes in scientific and engineering situations, differential equations have played a significant role in many scientific and engineering domains. Integral transforms are mathematical operations that convert a given function into a new representation, often in terms of a different variable or set of variables. These transforms are widely used in various branches of mathematics and physics to simplify the analysis and solution of complex problems. These problems involve finding the solution to a differential equation subject to certain boundary conditions. By applying an integral transform, the differential equation can be transformed into an equation involving the transform of the unknown function. This allows for the boundary conditions to be incorporated into the transformed equation, making it easier to find the solution. Lalit Mohan Upadhyaya[1] introduced the Upadhyaya transformation, a highly advanced transform

within the Laplace class, which holds great promise for cutting-edge applications across various fields of research. Upadhyaya and his colleagues[2] further developed this theory, positioning it as one of the most robust and sophisticated transforms in contemporary mathematics literature. Its potential spans disciplines including mathematics, engineering, physics, chemistry, biology, pharmaceuticals, economics, sociology, and more. Despite its vast potential, many applications of this transformative tool remain untapped. This paper focuses on demonstrating the application of the Upadhyaya transform in solving chemical kinetics problems, showcasing its efficacy within the realm of chemical sciences. Murphy[3] investigated consecutive chemical reactions of the first and second orders. Chrastil[4] used the final product to determine the rate constants of a first-order chemical process. Kalaiarasi *et al.,*[5] utilized the Kamal transform method to address Two Tank Mixing Problems, which involve solving first-order linear differential equations. To determine the concentration of chemical compounds, Higazy and Aggarwal[6] applied the Sawi transform to the mathematical model of the chemical reaction in series. Mousa[7] utilized the Upadhyaya transform to determine the solution for the Volterra integral equation of the first kind. Patil and others[8,9] applied the Soham and Kushare transforms in chemical sciences, while Peker *et al.,*[10] utilized the Kashuri Fundo Transform to obtain solutions for various chemical reaction models. To obtain the solution for Volterra integral equations of the second kind, Dinesh and Prakash[11] employed the Upadhyaya transform. Kuffi and Mansour[12] solved certain cardiovascular models using the Emad-Falih integr2al transform. Aggarwal *et al.,*[13] utilized the Rishi Transform to ascertain the concentrations of the chemical compounds in a first-order successive chemical reaction. Anuj *et al.,*[14] employed the Anuj transform to solve the problem of reactant concentrations in first-order successive chemical reactions analytically. To solve fractional integro-differential equations, Gunaseka and Prabakaran[15] used the Mohand transform. Recently, Dinesh and Kuffi[16] demonstrated the Upadhyaya transform's ability to solve ordinary differential equations by applying it to cardiovascular models. The present study highlights the significance of the Upadhyaya transform in solving chemical reaction models.

Definition of upadhyaya transform

The Upadhyaya transform of the function *f*(t)is mathematically defined as[1]:

$$U\{f(t)\} = \lambda_1 \int_0^{\infty} \exp(-\lambda_2 t) f(\lambda_3 t)\,dt = u(\lambda_1,\lambda_2,\lambda_3),\ (\lambda_1,\lambda_2,\lambda_3) > 0,\ t \geq 0 \quad (1)$$

The representation of the inverse Upadhyaya transform is as follows:

$$f(t) = U^{-1}\left[u(\lambda_1,\lambda_2,\lambda_3)\right],\ t \geq 0 \quad (2)$$

In the general formulation of the Upadhyaya transform, λ_1,λ_2 and λ_3 are complex parameters[1].

Some useful characteristics of upadhyaya transformation

Linearity property

If $f_1(t)$ be $f_2(t)$ two functions with UT's $u_1(\lambda_1, \lambda_2, \lambda_3)$ and $u_2(\lambda_1, \lambda_2, \lambda_3)$ in terms of the parameters λ_1, λ_2, λ_3 and b_1, b_2 be any constants then[1]

$$U[b_1 f_1(t) + b_2 f_2(t); \lambda_1,\lambda_2,\lambda_3] = b_1 U[f_1(t); \lambda_1,\lambda_2,\lambda_3] + b_2 U[f_2(t); \lambda_1,\lambda_2,\lambda_3] = b_1 u_1(\lambda_1,\lambda_2,\lambda_3) + b_2 u_2(\lambda_1,\lambda_2,\lambda_3).$$

Convolution property

If the Upadhyaya transform of the functions $f_1(t)$ and $f_2(t)$ with respect to the parameters λ_1, λ_2, λ_3 are $u_1(\lambda_1, \lambda_2, \lambda_3)$ and $u_2(\lambda_1, \lambda_2, \lambda_3)$ then convolution of Upadhyaya transform of the functions $f_1(t) * f_2(t)$ is given by[1]

$$U[f_1(t) * f_2(t); \lambda_1,\lambda_2,\lambda_3] = \frac{\lambda_3}{\lambda_1} u_1(\lambda_1,\lambda_2,\lambda_3) \cdot u_2(\lambda_1,\lambda_2,\lambda_3)$$

Where $f_1(t) * f_2(t)$ is given by

$$f_1(t) * f_2(t) = \int_0^t f_1(t-x) f_2(x)\,dx = \int_0^t f_1(x) f_2(t-x)\,dx$$

Upadhyaya transforms of some elementary functions[1]

$$U(1) = \frac{\lambda_1}{\lambda_2},\quad U(e^{at}) = \frac{\lambda_1}{\lambda_2 - a\lambda_3}, U(t^m) = \frac{m!\,\lambda_1\,\lambda_3^m}{\lambda_2^{m+1}} (m \in N)$$

$$U[\sin(at)] = \frac{a\lambda_1\lambda_3}{\lambda_2^2 + a^2\lambda_3^2}, U[\cos(at)] = \frac{\lambda_1\lambda_2}{\lambda_2^2 + a^2\lambda_3^2}$$

Upadhyaya transform of derivatives

$U[f_1(t)] = u(\lambda_1, \lambda_2, \lambda_3)$ If then from[1]

$$U[f'(t); \lambda_1,\lambda_1,\lambda_3] = \left(\frac{\lambda_2}{\lambda_3}\right) U[f(t); \lambda_1,\lambda_1,\lambda_3] - \frac{\lambda_1}{\lambda_3} f(0),$$

$$U[f''(t); \lambda_1,\lambda_2,\lambda_3] = \left(\frac{\lambda_2}{\lambda_3}\right)^2 U[f(t); \lambda_1,\lambda_2,\lambda_3] - \frac{\lambda_1\lambda_2}{\lambda_3^2} f(0) - \frac{\lambda_1}{\lambda_3} f'(0),$$

$$U[f^n(t); \lambda_1,\lambda_2,\lambda_3] = \left(\frac{\lambda_2}{\lambda_3}\right)^n U[f(t); \lambda_1,\lambda_2,\lambda_3] - \frac{\lambda_1\lambda_2^{n-1}}{\lambda_3^n} f(0) - \frac{\lambda_1\lambda_2^{n-2}}{\lambda_3^{n-1}} f'(0) - \frac{\lambda_1\lambda_2^{n-3}}{\lambda_3^{n-2}} f''(0) - \ldots\ldots - \frac{\lambda_1}{\lambda_3} f^{n-1}(0),$$

Applications of the upadhyaya transform in various chemical reaction models

In this section, we apply the Upadhyaya transform to solve several chemical reaction models represented by ordinary differential equations, which play a crucial role in the realm of chemistry.

The zero-order chemical reaction model satisfies the initial value problem[10]

$$\frac{dc(t)}{dt} = -k_0(t), t > 0, \quad (3)$$

$$c(0) = c_0 \quad (4)$$

where

c(t)– concent ration of reacting substance at time t, k_0-positive constant.

Performing the Upadhyaya transform bilaterally in equation (3) yields

$$U\left[\frac{dc(t)}{dt}\right] = U[-k_0(t)] \quad (5)$$

Let U[*c(t)*] = u*(*$\lambda_1, \lambda_2, \lambda_3$*)* Using the derivative property of Upadhyaya transform and initial condition (4), we obtain equation (6)

$$u(\lambda_1, \lambda_2, \lambda_3) = c_0 \times \frac{\lambda_1}{\lambda_2} - k_0 \frac{\lambda_1 \lambda_3}{\lambda_2^2} \quad (6)$$

After applying bilaterally the inverse Upadhyaya transform to equation (6), we will find the solution to the given initial value problem as

$$c(t) = c_0 - k_0 t \quad (7)$$

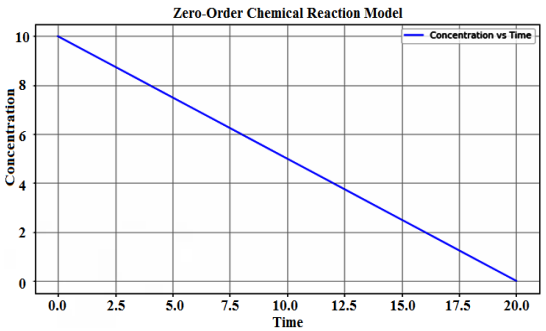

Fig. 1. The solution behaviour of application 4.1.

Figure 1 illustrates the concentration of a reacting substance over time in a zero-order chemical reaction. Starting from an initial concentration (c_0), the concentration decreases linearly with time, indicating a constant reaction rate. The slope of the graph represents the rate constant (k_0), with a negative value denoting a decrease in concentration over time. This linear decrease in concentration showcases the characteristic behavior of zero-order reactions, where the rate remains unaffected by changes in concentration.

The First-order chemical reaction model satisfies the initial value problem[10]

$$\frac{dc(t)}{dt} = -k_1 c(t), k_1 > 0 \quad (8)$$

$$c(0) = c_0 \quad (9)$$

We apply the Upadhyaya transform to solve the given first-order chemical reaction model.

Applying the Upadhyaya transform bilaterally to equation (8) yields

$$U\left[\frac{dc(t)}{dt}\right] = U[-k_1 c(t)] \quad (10)$$

Let *U*[*c(t)*] = u*(*λ_1, λ_2, λ_3*)*By rearranging equation (10) in accordance with the initial condition (9) and Upadhyaya transform's derivative property, we obtain

$$u(\lambda_1, \lambda_2, \lambda_3) = c_0 \frac{\lambda_1}{\lambda_2 + k_1 \lambda_3} \quad (11)$$

After applying bilaterally the inverse Upadhyaya transform to equation (11), we will find the solution to the given initial value problem as

$$c(t) = c_0 e^{-k1t} \quad (12)$$

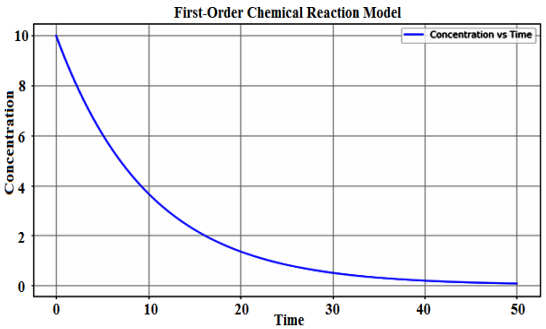

Fig. 2. The solution behaviour of application 4.2

Figure 2 depicts the concentration of a reacting substance over time in a first-order chemical reaction. As time progresses, the concentration exponentially decreases, following a decay curve

characterized by the rate constant (k_1), The initial concentration (c_0), determines the starting point of the curve, with higher initial concentrations leading to slower decay rates.

Now we determine the solutions for the systems of differential equations that govern the successive chemical reactions of the first order given by[10]

$$\frac{dc_1(t)}{dt} = -k_1 c_1(t),\ \frac{dc_2(t)}{dt} = k_1 c_1(t) - k_2 c_2(t)\ ,\frac{dc_3(t)}{dt} = k_2 c_2(t)\ , t > 0 \quad (13)$$

With the initial conditions

$$c_1(0)=c_0,\ c_2(0) = c_3(0) = 0 \quad (14)$$

In equation (2), $c_1(t)$ is the concentration of substance *A1* at time *t*, which breaks down to generate the new substance *A2* with concentration $c_2(t)$, and $c_3(t)$ is the concentration of a new element derived from.

In the prior application, we determined that the differential equation of the function $c_1(t)$ has a solution as $c_0 e^{-k1t}$. When we plug $c_0 e^{-k1t}$ solution into the differential equation of the $c_2(t)$ function, we get

$$\frac{dc_2(t)}{dt} = k_1 c_0 e^{-k_1 t} - k_2 c_2(t) \quad (15)$$

Applying the Upadhyaya transform bilaterally to equation (15) yields

$$U\left[\frac{dc_2(t)}{dt}\right] = k_1 c_0 U[e^{-k_1 t}] - k_2 U[c_2(t)] \quad (16)$$

Let $U[c_2(t)] = u(\lambda_1, \lambda_2, \lambda_3)$. By rearranging equation (16) in accordance with the initial condition (14) and Upadhyaya transform's derivative property, we obtain

$$u(\lambda_1, \lambda_2, \lambda_3) = \frac{k_1 c_0}{k_2 - k_1}\left[\frac{\lambda_1}{\lambda_2 + k_1\lambda_3} - \frac{\lambda_1}{\lambda_2 + k_2\lambda_3}\right] \quad (17)$$

After applying bilaterally the inverse Upadhyaya transform to equation (17), we get

$$c_2(t) = \frac{k_1 c_0}{k_2 - k_1}\left[e^{-k_1 t} - e^{-k_2 t}\right] \quad (18)$$

We now have the solutions to the differential equation of the function $c_2(t)$. Substituting $c_2(t) = \frac{k_1 c_0}{k_2 - k_1}[e^{-k_1 t} - e^{-k_2 t}]$ into the differential equation for the function produces the following result:

$$\frac{dc_3(t)}{dt} = \frac{k_2 k_1 c_0}{k_2 - k_1}\left[e^{-k_1 t} - e^{-k_2 t}\right] \quad (19)$$

Applying the bilateral Upadhyaya transform to equation (19), we obtain

$$U\left[\frac{dc_3(t)}{dt}\right] = \frac{k_2 k_1 c_0}{k_2 - k_1}\left[U(e^{-k_1 t}) - U(e^{-k_2 t})\right] \quad (20)$$

Let $U[c_3(t)] = u(\lambda_1, \lambda_2, \lambda_3)$ and using the derivative property of Upadhyaya transform, we obtain

$$\frac{\lambda_2}{\lambda_3}u(\lambda_1, \lambda_2, \lambda_3) - \frac{\lambda_1}{\lambda_3}c_3(0) = \frac{k_2 k_1 c_0}{k_2 - k_1}\left[\frac{\lambda_1}{\lambda_2 + k_1\lambda_3} - \frac{\lambda_1}{\lambda_2 + k_2\lambda_3}\right] \quad (21)$$

Equation (21) can be expressed as follows by using the initial condition (14).

$$u(\lambda_1, \lambda_2, \lambda_3) = \frac{\lambda_3}{\lambda_2} \times \frac{k_2 k_1 c_0}{k_2 - k_1}\left[\frac{\lambda_1}{\lambda_2 + k_1\lambda_3} - \frac{\lambda_1}{\lambda_2 + k_2\lambda_3}\right] \quad (22)$$

Rearranging the equation (22), we get

$$u(\lambda_1, \lambda_2, \lambda_3) = c_0\frac{\lambda_1}{\lambda_2} - c_0\frac{\lambda_1}{\lambda_2 + k_1\lambda_3} - \frac{k_1 c_0}{k_2 - k_1}\left[\frac{\lambda_1}{\lambda_2 + k_1\lambda_3} - \frac{\lambda_1}{\lambda_2 + k_2\lambda_3}\right] \quad (23)$$

After applying bilaterally the inverse Upadhyaya transform to equation (23), we get

$$c_3(t) = c_0 - c_0 e^{-k_1 t} - \frac{k_1 c_0}{k_2 - k_1}\left[e^{-k_1 t} - e^{-k_2 t}\right] \quad (24)$$

Considering the previous solutions, the outcome can alternatively be stated as follows:

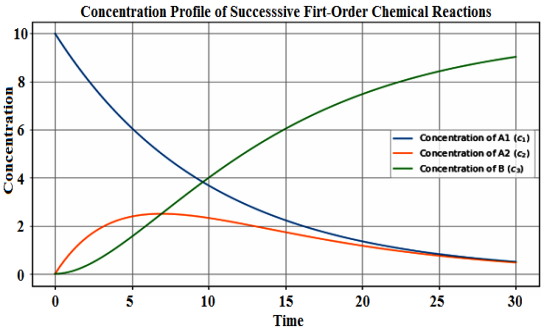

Fig. 3. The solution behaviour of application 4.3

Figure 3 depicts the evolution of concentrations in a system undergoing successive first-order chemical reactions. Initially, the concentration *A1*(c_1) of is high and gradually decreases exponentially over time as it transforms into *A2*(c_2). A2's concentration rises initially, reaching a plateau as it accumulates, then slowly declines. Meanwhile, B's concentration (c_3) steadily increases over time as it forms from A2, eventually leveling

off. This dynamic interplay among the substances highlights the intricate kinetics of first-order reactions and the transformation of reactants into products.

CONCLUSION

This research showcases how employing the Upadhyaya transform for chemical reaction models has proven to be effective and elegant, streamlining the solution process of ordinary differential equations commonly encountered in chemical kinetics and various other branches of chemistry. By providing a streamlined approach that requires minimal computational burden, this transform offers a valuable tool for researchers and practitioners in understanding reaction kinetics. The inclusion of graphical representations has further enhanced the interpretability of results, facilitating deeper insights into the temporal evolution of reactant concentrations. Moving forward, there is potential for extending the utility of the Upadhyaya transform to more complex chemical systems and exploring its integration with advanced computational techniques for real-time simulation and optimization. This underscores its significance as a versatile method with promising implications for advancing our understanding and application of chemical kinetics.

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Conflict of interest

The authors declare no conflict of interest.

REFERENCES

1. Upadhyaya, L. M. Introducing the Upadhyaya integral transform. *Bulletin of Pure and Applied Sciences, Section E (Mathematics and Statistics).,* **2019**, *38E*(1), 471–510.
2. Upadhyaya, L. M.; Shehata, A.; Kamal, A. An update on the Upadhyaya transform., *Bulletin of Pure and Applied Sciences, Section E (Mathematics and Statistics).,* **2021**, *40E*(1), 26-44.
3. Murphy, R. D. Exact solution of rate equations for consecutive first and second order reactions., *Indian Journal of Chemistry*., **1993**, *32A*, 381-382.
4. Chrastil, J. Determination of the first order consecutive reaction rate constants from final product., *Computers & Chemistry*., **1988**, *12*(4), 289-292.
5. Kalaiarasi, S.; Keerthana, S.; Nithiyapriya, N.; Anita, M. Applications of Kamal transform in two tank mixing problems., *Advances in Mathematics: Scientific Journal*., **2020**, *9*(8), 5927–5934.
6. Higazy, M.; Aggarwal, S. Sawi transformation for system of ordinary differential equations with application., *Ain Shams Engineering Journal*., **2021**, *12*(3), 3173-3182.
7. Mousa, Adil. Application of the Upadhyaya transform to Volterra integral equations of the first kind., *Bulletin of Pure and Applied Sciences, Section E (Mathematics and Statistics).,* **2021**, *40E*(2), 140-148.
8. Patil, D. P.; Wagh, P. S.; Wagh, P. Applications of Soham Transform in Chemical Sciences., *International Journal of Science, Engineering and Technology*., **2022**, *10*(3), 1-5.
9. Patil, D. P.; Wagh, P. S.; Wagh, P. Applications of Kushare Transform in Chemical Sciences., *International Journal of Science, Engineering and Technology*., **2022**, *10*(3).
10. Peker, H. A.; Cuha, F. A.; Peker, B. Kashuri Fundo transform for solving chemical reaction models. In Proceedings of the International E-Conference on Mathematical and Statistical Sciences: *A Selcuk Meeting, Konya, Turkey*., **2022**, 20-22.
11. Thakur, D.; Thakur, P.C. Utilizing the Upadhyaya Transform to Solve the Linear Second Kind Volterra Integral Equation., *The Review of Contemporary Scientific and Academic Studies*., **2023**, *3*(4), 1-6.
12. Mansour, E. A.; Kuffi, E. A. The Utilization of the Emad-Falih Integral transformation to solve some cardiovascular models., *Mathematics for Applications-Submission Portal*., **2023**, *12*(2), 18-21.

13. Aggarwal, S.; Kumar, R.; Chandel, J. Rishi Transform for Determining the Concentrations of the Chemical Compounds in First Order Successive Chemical Reaction., *Journal of Advanced Research in Applied Mathematics and Statistics*., **2023**, *8*(1&2), 10-17.
14. Kumar, A.; Bansal, S; Aggarwal, S. Determination of the concentrations of the reactants of first order consecutive chemical reaction using Anuj transform., *European Chemical Bulletin*., **2023**, *12*(7), 2528-2534.
15. Gunasekar, T.; Raghavendran, P. The Mohand transform approach to fractional integro-differential equations., *Journal of Computational Analysis and Applications.,* **2024**, *33*(1), 358-371.
16. Thakur, D; Kuffi, E.A. Exact solutions of Cardiovascular Models by using Upadhyaya transform., *Journal of Kufa for Mathematics and Computer*., **2024**, *11*(1), 37-42.