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Implementation of Fractional Blood Ethanol Model by Computation of Matrix Mittag–Leffler Functions

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Abstract

The article discusses several innovative and intriguing aspects of the fractional operator-based fractional blood ethanol concentration model involving first-order chemical reactions. The most commonly used fractional operator, Caputo, performs the analysis. The analytical results of blood ethanol concentration are examined utilizing the computation matrix Mittag-Leffler function (MMLF). Solutions' ethanol concentrations are displayed as an extended series. A graphical representation of the effect of fractional parameters on ethanol concentrations is provided. The comparative analysis for concentrations demonstrates the proposed model's novel composite fractional derivative properties. According to studies, fractional models approximate real data more correctly than their integer order derivative operator counterparts. The fractional blood alcohol models presented provide essential and beneficial results that can be used to forecast future information for the medical community.

Keywords: Caputo fractional derivative, Fractional blood ethanol model, Mittag-Leffler, computation matrix Mittag-Leffler function.
2010 MSC: 26A33, 33F05, 34A08, 92B05.

1. Introduction

The pace of a reaction indicates how quickly the concentration or pressure of the chemicals involved in it changes as a result of the response. The number of reactants present, their surface area, pressure, activation energy, temperature, and other factors affects how quickly it proceeds. Chemical kinetics, often known as "reaction kinetics," has

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rapidly advanced with current chemical and industrial expertise. These activities depend on medical research, engineering, geothermal reservoirs, food processing, oil reservoirs, and the chemical sector. Modern times have seen a significant increase in the industrial sector's interest in the intensive study of reaction kinetics, which was previously only a laboratory topic.

Chemical kinetics research on reactions reveals essential details about changes affecting a person's daily life. It explains how chemical reactions produce new compounds from available reactants. Knowing how quickly specific tablets function, how quickly food spoils, how quickly fruits-vegetables produce rots, how rapidly carbon steel oxidizes, and many other related processes occur is attractive to everyone. The reaction rate is affected by the type of reactants, the surrounding temperature, the presence/absence of a catalyst, and several different factors. The rule of mass action enables us to establish rate laws and chemical kinetic rate constants, and it is often used to compute reaction rates from investigational data. As a result, it is feasible to determine the reaction's speed and how the chemical compound;s concentrations influence it. Ludwin [9] experimentally established the alcohol concentration in human blood. One such rate law equation is looked at in the current work to explore the current work examines one such rate law equation to explore the implications of considering fractional order rates of change.

The study of fractional calculus and its results has drawn the attention of many academics in the modern period; it may explain the most excellent outcomes applicable to everyday life. Several academics proposed definitions of differential and integral operators in fractional calculus, which are crucial to the current work. Researchers, scientists, and practitioners are also fascinated by the capacity to model differential equations as a function of time. As they are more suitable than traditional conventional models based on integer order derivatives and integrals, fractional derivative and integral-based mathematical models have grown in favor among scientists throughout time. Fractional calculus has many applications in applied mathematics and fields like medical science, engineering, physics, economics, chemistry, finance, and even social science [3, 11, 12, 15]. The RL (Riemann-Liouville) and Caputo's classical definitions are the two definitions of fractional derivatives most often utilized. This study establishes a blood ethanol model based on the Caputo operator and solves it using the computation matrix Mittag-Leffler function.

Ludwin [9] conducted an experimental investigation to ascertain the amount of alcohol present in the human body's stomach $\mathscr{Z}_1(t)$ and blood $\mathscr{Z}_2(t)$. It is the primary source for the current research study's real data. The fundamental integer order model is based on a first order kinetic process as defined by

$$\begin{aligned} \frac{d\mathscr{Z}_1(t)}{dt} &= -\sigma\mathscr{Z}_1(t), \\ \frac{d\mathscr{Z}_2(t)}{dt} &= \sigma\mathscr{Z}_1(t) - \kappa\mathscr{Z}_2(t), \end{aligned} \tag{1.1}$$

where $\mathscr{Z}_1(t)$ is the amount of ethanol in the stomach at any given time (t), $\mathscr{Z}_2(t)$ is the amount of ethanol in the blood at the same time (t), σ and κ are rate law constants. The following are the beginning conditions for the model above:

$$\mathscr{Z}_1(0) = \zeta_1, \text{ and } \mathscr{Z}_2(0) = \zeta_2. \tag{1.2}$$

The primary objective of this paper is to examine the fractional version (utilizing the Caputo operator) of a mathematical model originally formulated with integer-order operators for the design of first-order kinetic reactions in the field of chemical engineering. Additionally, the utilization of real-world data contributes to a clearer comprehension of the analysis involving fractional operators. The behavior of the fractional model's exact solution in comparison to the outcomes of the initial integer order model is another goal of the article. Finally, to make the present study understandable to a wide range of readers, we calculated the sum of squared residuals to gain useful insights within the fractional volumes. It is important to highlight that the fractional version of the model underwent previous consideration in ref under the Caputo, ABC, and CF operators [1, 2, 7], which is relevant to the current investigation. This distinction lies in considering dimensional stability, a factor previously overlooked in earlier studies. This inclusion has proven instrumental in attaining precise solutions for the partial models discussed in pertinent literature. Furthermore, the analysis incorporates real data on blood alcohol content in the human body, sourced from actual observations [9], to evaluate the results obtained under the Caputo operator.

The structure of this paper is arranged as follows: Section 2 introduces essential definitions and explores integral transforms associated with key fractional operators. Section 3 is devoted to the' analytical treatment and solution of fractional differential equations. In Section 4, we provide the numerical implementation along with graphical illustrations. Finally, Section 5 concludes the study with a summary of findings.

2. Mathematical groundwork

This section outlines the core mathematical concepts and notations that serve as the foundation for the analysis carried out in this study. It includes essential definitions and commonly used fractional calculus operators, crucial in formulating and solving the fractional models addressed in later sections. A clear understanding of these tools is vital for grasping the work's theoretical and numerical aspects.

Below, we present some of the key mathematical terms and operators used in this research:

Definition 2.1. The following Mittag–Leffler (ML) functions, $E_\rho(\mathscr{G})$ and $E_{\rho,\tau}(\mathscr{G})$, were introduced by Mittag-Leffler [10] and Wiman [16], respectively.

$$E_\rho(\mathscr{G}) = \sum_{k=0}^{\infty} \frac{\mathscr{G}^k}{\Gamma(\rho k+1)} \; ; \quad \big(\mathscr{G}, \rho \in \mathbb{C}, \Re(\rho) > 0\big),$$

and

$$E_{\rho,\tau}(\mathscr{G}) = \sum_{k=0}^{\infty} \frac{\mathscr{G}^k}{\Gamma(\rho k+\tau)} \; ; \quad \big(\mathscr{G}, \rho, \tau \in \mathbb{C}, \Re(\rho) > 0, \Re(\tau) > 0\big).$$

Definition 2.2. The standard definition of the RL fractional integral [14] of ϕ of order $\Re(\nu) > 0$ is given as follows:

$${}_b\mathbb{I}_y^\nu \phi(y) = \frac{1}{\Gamma(\nu)} \int_b^y (y-\xi)^{\nu-1} \phi(\xi) d\xi.$$

Definition 2.3. The standard CFD (Caputo fractional derivative) of order $\vartheta \in (0,1)$ is determined by [8] ,

$$ {}^{C}\mathfrak{D}_{s}^{\vartheta}[\phi(s)] = \frac{1}{\Gamma(l-\vartheta)} \int_{0}^{s} \frac{\phi^{l}(z)}{(s-z)^{\vartheta-l+1}}\, dz, $$

where $l = [\vartheta] + 1$.

3. Solution of a system of equivalent order FDE

Although integer order equations give some successful results, it is clear that FDEs give more realistic results to real phenomena than integer order equations. The main feature distinguishing FDEs from integer sequences is the non-local property of FDEs not found in integer differential equations. This phenomenon can be successfully reflected using FDEs. Furthermore, FDEs reduce errors caused by parameters that we ignore while modeling. Because of these valuable features of FDEs, various models have been studied using fractional-order differential equations [13, 5, 6]. In fractional systems, dimensional consistency is an essential tool in which the units of measurement from the left and right sides of the equations are consistent. This stability can be provided by modifying the parameters on the right-hand side of the equations, for example, by raising them to the power δ. In this context, we have extended the model given in (1.1) to fractional order in the Caputo sense, which is presented in the following system:

$$ \begin{aligned} \mathfrak{D}_{t}^{\delta}\mathscr{Z}_{1}(t) &= -\sigma^{\delta}\mathscr{Z}_{1}(t), \\ \mathfrak{D}_{t}^{\delta}\mathscr{Z}_{2}(t) &= \sigma^{\delta}\mathscr{Z}_{1}(t) - \kappa^{\delta}\mathscr{Z}_{2}(t), \end{aligned} \tag{3.1} $$

assuming $\sigma^{\delta} = \beta$ and $\kappa^{\delta} = \omega$, Equation (3.1) can be simplified to Equation (3.2).

$$ \begin{aligned} \mathfrak{D}_{t}^{\delta}\mathscr{Z}_{1}(t) &= -\beta\mathscr{Z}_{1}(t), \\ \mathfrak{D}_{t}^{\delta}\mathscr{Z}_{2}(t) &= \beta\mathscr{Z}_{1}(t) - \delta\mathscr{Z}_{2}(t). \end{aligned} \tag{3.2} $$

Think about the IVP (initial value problem) of FDE (3.2)

$$ \mathfrak{D}_{t}^{\delta}\mathscr{Z}(t) = M\mathscr{Z}(t), \quad t > 0, \tag{3.3} $$

where

$$ M = \begin{bmatrix} -\beta & 0 \\ \beta & -\omega \end{bmatrix}, \quad 0 < \delta \leqslant 1, $$

the initial condition $\mathscr{Z}(0) = (\zeta_1, \zeta_2)^{T}$ is included, and the CFD $\mathfrak{D}_{t}^{\delta}\mathscr{Z}(t)$ is employed componentwise, i.e., $\mathfrak{D}_{t}^{\delta}\mathscr{Z}(t) = (\mathfrak{D}_{t}^{\delta}\mathscr{Z}_{1}(t), \mathfrak{D}_{t}^{\delta}\mathscr{Z}_{2}(t))^{T}$. We apply the Picard iterative technique to determine the IVP series solution. Using the integral operator $\mathfrak{I}_{t}^{\delta}$ in conjunction with Equation (3.3) and the expression $\mathfrak{I}_{t}^{\delta}\mathfrak{D}_{t}^{\delta}\mathscr{Z}(t) = \mathscr{Z}(t) - \mathscr{Z}(0)$, we obtain

$$ \mathscr{Z}(t) = \mathscr{Z}(0) + M\mathfrak{I}_{t}^{\delta}\mathscr{Z}(t). $$

The ℓth approximate solution is designated by the $\Phi_{\ell}(t)$, where the zeroth approximate solution has been determined as

$$ \Phi_{0}(t) = \mathscr{Z}(0). $$

The recurrence formula holds for $\ell \geqslant 1$,

$$\Phi_\ell(t) = \mathscr{Z}(0) + M\mathfrak{I}_t^\delta \Phi_{\ell-1}(t).$$

We do sequential computations using the recurrent formula.

$$\begin{aligned}
\Phi_1(t) &= \mathscr{Z}(0) + \frac{Mt^\delta}{\Gamma(\delta+1)}\mathscr{Z}(0),\\
\Phi_2(t) &= \mathscr{Z}(0) + \frac{Mt^\delta}{\Gamma(\delta+1)}\mathscr{Z}(0) + \frac{M^2t^{2\delta}}{\Gamma(2\delta+1)}\mathscr{Z}(0),\\
&\cdots,\\
\Phi_\ell(t) &= \sum_{\hbar=0}^{\ell} \frac{M^\hbar t^{\hbar\delta}}{\Gamma(\hbar\delta+1)}\mathscr{Z}(0).
\end{aligned}$$

By using the limit $\ell \to \infty$ for $\Phi_\ell(t)$, we deduce the series expression for a solution.

$$\Phi_\ell(t) = \sum_{\hbar=0}^{\infty} \frac{M^\hbar t^{\hbar\delta}}{\Gamma(\hbar\delta+1)}\mathscr{Z}(0).$$

The solution takes the form of a matrix ML function

$$\mathscr{Z}(t) = E_{\delta,1}(Mt^\delta)\mathscr{Z}(0).$$

Following is a technique for computing the MMLF $E_{\delta,\tau}(Mt^\delta)$, where the MMLF are represented by matrix polynomials with coefficients expressed in terms of the scalar MLF $E_{\delta,\tau}(\xi t^\delta)$.

The eigenvalues of the matrix M are $\xi_1 = -\beta$ and $\xi_2 = -\omega$. By utilizing the Jordan canonical form $M = PJP^{-1}$, where

$$P = \begin{bmatrix} \frac{\omega-\beta}{\beta} & 0 \\ 1 & 1 \end{bmatrix}, \text{ and } J = \begin{bmatrix} \xi_1 & 0 \\ 0 & \xi_2 \end{bmatrix},$$

Thus, from the matrix theory [4], we have

$$E_{\delta,\tau}(Mt^\delta) = P \begin{bmatrix} E_{\delta,\tau}(\xi_1 t^\delta) & 0 \\ 0 & E_{\delta,\tau}(\xi_2 t^\delta) \end{bmatrix} P^{-1}, \tag{3.4}$$

Alternatively, using the familiar Lagrange-Sylvester interpolation polynomial, $E_{\delta,\tau}(Mt^\delta)$ may be uniquely expressed as a matrix polynomial of degree one.

In the current scenario, we consider the polynomial

$$a_0(t) + a_1(t)\xi = \phi(\xi; t),$$

with $\phi(M; t) = E_{\delta,\tau}(Mt^\delta)$ and the function $E_{\delta,\tau}(\xi t^\delta)$ be identical in the spectrum of matrix M, we have

$$\begin{aligned}
a_0(t) + a_1(t)\xi_1 &= E_{\delta,\tau}(\xi_1 t^\delta),\\
a_0(t) + a_1(t)\xi_2 &= E_{\delta,\tau}(\xi_2 t^\delta).
\end{aligned}$$

The system solution leads to

$$a_0(t) = \frac{\beta\, E_{\delta,\tau}(\xi_2 t^\delta) - \omega\, E_{\delta,\tau}(\xi_1 t^\delta)}{\beta - \omega},$$
$$a_1(t) = \frac{E_{\delta,\tau}(\xi_2 t^\delta) - E_{\delta,\tau}(\xi_1 t^\delta)}{\beta - \omega}.$$

As a result, the MMLF has the form

$$E_{\delta,\tau}(Mt^\delta) = \left[\frac{\beta}{\beta-\omega}E_{\delta,\tau}(\xi_2 t^\delta) - \frac{\omega}{\beta-\omega}E_{\delta,\tau}(\xi_1 t^\delta)\right] I_{2\times 2} + \left[\frac{E_{\delta,\tau}(\xi_2 t^\delta)}{\beta-\omega} - \frac{E_{\delta,\tau}(\xi_1 t^\delta)}{\beta-\omega}\right] M. \tag{3.5}$$

We tested the consistent nature of Equations (3.4) and (3.5) findings.

The outcome of Equation (3.3)'s IVP, parameterized by the order δ is

$$\begin{aligned}\mathscr{Z}(t) &= E_{\delta,1}(Mt^\delta)\mathscr{Z}(0)\\ &= \left[\left[\frac{\beta}{\beta-\omega}E_{\delta,1}(\xi_2 t^\delta) - \frac{\omega}{\beta-\omega}E_{\delta,1}(\xi_1 t^\delta)\right] I_{2\times 2} + \left[\frac{E_{\delta,1}(\xi_2 t^\delta)}{\beta-\omega} - \frac{E_{\delta,1}(\xi_1 t^\delta)}{\beta-\omega}\right] M\right]_{2\times 2} \mathscr{Z}(0).\end{aligned}$$

4. Numerical computation and graphical discussion

In this section, we implement the matrix Mittag-Leffler to get numerical results of the fractional order alcohol model of Equation with: $\zeta_1 = 373,\ \zeta_2 = 0,\ \sigma = 0.064,\ \kappa = 0.008$.

$$\mathscr{Z}_1(t) = \zeta_1 \sum_{\ell=0}^{\infty} \frac{(-\beta t^\delta)^\ell}{\Gamma(\ell\delta+1)},$$
$$\mathscr{Z}_2(t) = \zeta_1 \frac{\beta}{\beta-\omega} \sum_{\ell=0}^{\infty} \frac{t^{\delta\ell}}{\Gamma(\ell\delta+1)}\left((-\omega)^\ell - (-\beta)^\ell\right).$$

A glance at Figure 1 reveals that the Caputo operator takes the longest to lower the quantity of alcohol in a person's stomach. Figure 1 demonstrates that the Caputo and Integer order solution curves are similar to the real data implemented. Figure 2 displays the quantity of alcohol in a human's blood and stomach over time at various fractional orders. Table 1 shows the real data and the data derived from the model's precise answer for each case. The sum of squared residuals reveals that the Caputo fractional operator has a very small minimum error.

Additionally, it is noted that using the Caputo operator instead of the original integer order model, correct data may now be predicted with an accuracy of around 18.14% higher.

$$\frac{\text{SSE (Integer order)} - \text{SSE (CFD)}}{9} = 1.81355 \times 10^{-1}.$$

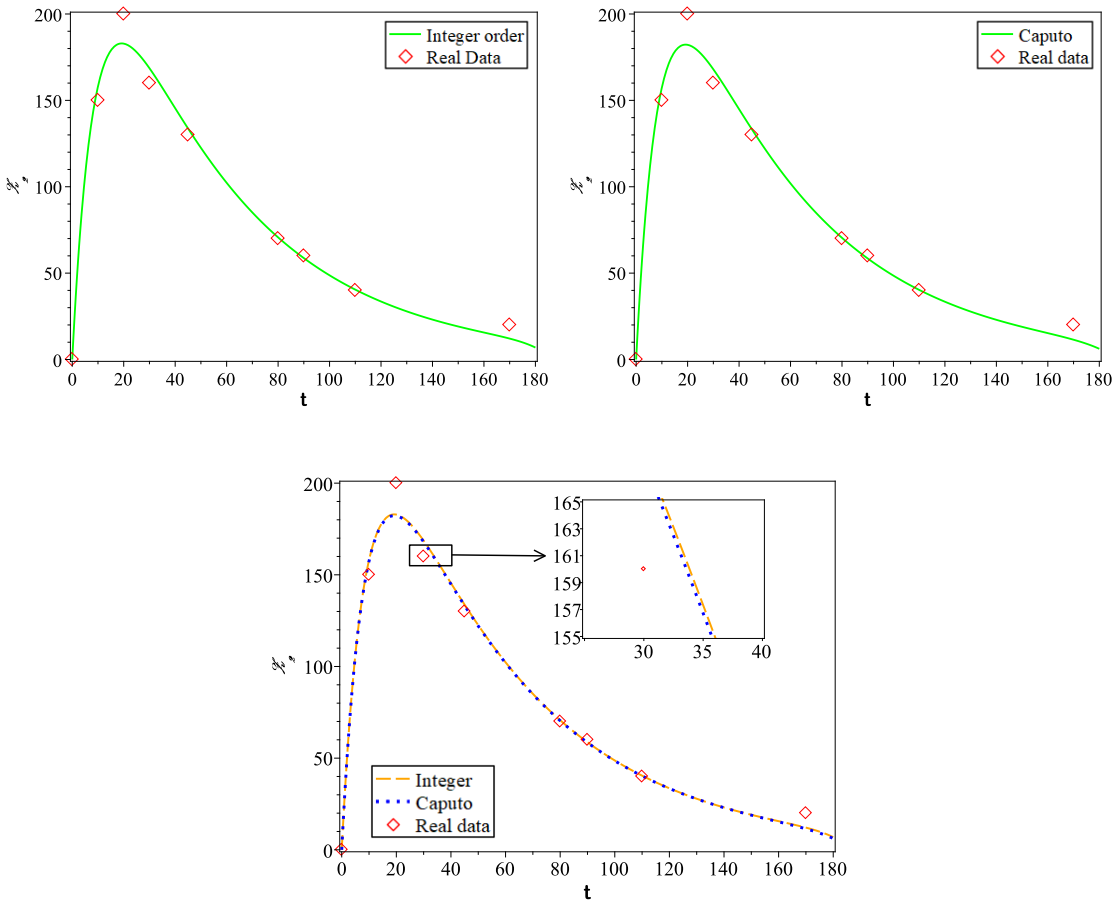

Figure 1: Comparison between real-world data and simulation results obtained from integer-order and fractional-order models, illustrating the amount of alcohol in the human bloodstream over time.

Time	**0**	**10**	**20**	**30**	**45**
Real [9]	0	150	200	160	130
Integer	0	1.58107×10^{2}	1.82848×10^{2}	1.68620×10^{2}	1.33734×10^{2}
CFD	0	1.57502×10^{2}	1.82150×10^{2}	1.67975×10^{2}	1.33223×10^{2}

Time	**80**	**90**	**110**	**170**
Real [9]	70	60	40	20
Integer	7.06949×10^{1}	5.86992×10^{1}	4.04484×10^{1}	1.32275×10^{1}
CFD	7.04247×10^{1}	5.84749×10^{1}	4.02939×10^{1}	1.31770×10^{1}

Table 1: Data from the integer and fractional order models are compared to data from actual blood alcohol concentrations.

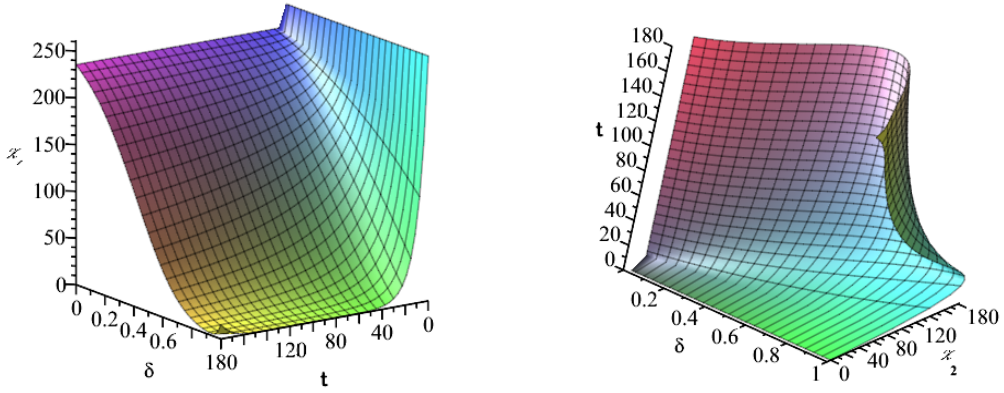

Figure 2: Human blood and stomach alcohol levels in different fractional orders over time.

We observe that the model under consideration has demonstrated satisfactory accuracy in predicting concentration at a given time, as evident from theoretical considerations and well-supported numerical results. However, it is essential to acknowledge that the discussed fractional model possesses certain limitations in its predictive capacity and overall adequacy. The constants utilized in the model exhibit variability across subjects, being influenced by factors such as stomach size, weight, blood quantity, liver function, and various other potential variables specific to the individual. In a precise context, our observations indicate that the discussed fractional model produces valuable and meaningful results, contributing to the interpolation of new information within a medical context. Further research is warranted to assess its accuracy across a broader population.

5. Conclusions and future biological implications

A system is partially partitioned under the Caputo operator for a first-order kinetic reaction in chemistry while considering the model's dimensionality. Comparing accurate data, integer order, and Caputo operators reveals that operators with and without singu-

larity (especially Caputo) are more appropriate for the numerical modeling of the system under consideration in the current research work. Using accurate data, it has been demonstrated that the fractional version of the model based on the Caputo operator can predict human blood alcohol content more accurately than the integer order version. Additionally, the optimal match of parameters δ displays the fractional behavior of alcohol concentration in the human stomach. In contrast, the behavior conforms to a traditional first-order kinetic response to the blood alcohol concentration.

Applying the numerical findings of this study in a medical environment could enhance the precision of understanding peak plasma concentration. One potential approach involves dividing time intervals into distinct functions to develop a more accurate approximation. Additionally, incorporating specific individual parameters such as blood quantity, weight, and stomach size into the simulation could further improve accuracy. In summary, a comprehensive consideration of the essential findings discussed across all sections and concluding remarks would be valuable for medical professionals and researchers in evaluating the implications of blood ethanol details. The fractional model explored in this paper demonstrates fundamental and beneficial outcomes, offering valuable insights for the interpolation of novel information in the medical field. Further research is encouraged to assess its accuracy across a broader population.

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Ethical Approval

No personal or sensitive information is disclosed or compromised.

Availability of Data and Access

No data were generated or analysed during this study.

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