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EDITED BY

Akif Akgul,
Hitit University, Türkiye

REVIEWED BY

Ahmed Elaiw,
King Abdulaziz University, Saudi Arabia
Yusuf Alaca,
Hitit University, Türkiye
Mahfud Mahfud,
Sepuluh Nopember Institute of
Technology, Indonesia

*CORRESPONDENCE

Fahad Al Basir
✉ fahadbasir@gmail.com
Priti Kumar Roy
✉ pritiju@gmail.com

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Optimization of biodiesel synthesis using ultrasound and mechanical stirring methods: a comparative study

Sk Mosaraf Ahammed¹, Amit Kumar Roy¹, Xue-Zhi Li²,
Fahad Al Basir^{3*} and Priti Kumar Roy^{1*}

¹Center of Mathematical Biology and Ecology, Department of Mathematics, Jadavpur University, West Bengal, Kolkata, India, ²School of Mathematics and Statistics, Henan Normal University, Xinxiang, China, ³Department of Mathematics, Asnasol Girls' College, West Bengal, India

Mechanical stirring (MS) and ultrasound (US) frequency are two key factors commonly used to reduce mass-transfer resistance during the reaction between methanol (MeOH) and triglycerides (TG), facilitating the efficient production of biodiesel (BD) from various feedstocks such as rapeseed oil and *Jatropha curcas* oil. In this study, a comparative model analysis has been conducted to evaluate the performance efficacy of optimum mechanical stirring (MS) and optimum ultrasound (US) frequency using rapeseed oil biodiesel production. Sensitivity and uncertainty analyses have been conducted using Latin hypercube sampling (LHS) and Partial Rank Correlation Coefficients (PRCCs) to identify the key kinetic and transport parameters influencing biodiesel yield. An optimal control framework has also been applied to regulate MS speed and US frequency over time to overcome initial mass-transfer resistance between oil and methanol. The influence of mixing intensity on biodiesel conversion has been examined at different temperatures and MeOH:oil molar ratios using mass-transfer correlations for both MS and US frequency. Numerical results show that, at a MeOH:TG molar ratio of 6:1 and temperature of 50 °C, optimal US frequency achieves a maximum biodiesel conversion of 97.67% within 40 min, whereas optimal MS attains 95.32% conversion after 60 min. The results further indicate that ultrasound provides faster mass-transfer enhancement and a superior production profile compared to mechanical stirring. This study addresses two key questions: whether rapeseed oil is a suitable feedstock for biodiesel production, and which mixing strategy, MS or US frequency, more effectively minimizes the mass-transfer resistance over time.

KEYWORDS

biodiesel production, Latin hypercube sampling (LHS), mathematical model, optimal control theory, sensitivity analysis (PRCCs)

1 Introduction

Biodiesel (BD) is widely recognized as a promising substitute owing to its sustainability, environmental friendliness, and ability to mitigate resource depletion during production [1]. Biodiesel combustion typically leads to lower emissions of harmful gases and particulates compared to conventional petroleum diesel, reducing CO₂ by 50%–80%, CO by 48%–50%, particulate matter by 30%–50%, and hydrocarbons by 67% [2, 3]. Various feedstocks such as vegetable

oils (palm oil, rapeseed oil, *Jatropha curcas* oil, soybean oil, etc.), animal fats, and recycled cooking oils can be used to produce biodiesel via a transesterification reaction. The oil or fat reacts with an alcohol, typically methanol (MeOH), in the presence of a catalyst, forming biodiesel and glycerol. *J. curcas* oil is favored for biodiesel production due to its non-edible nature and its ability to be cultivated on marginal lands. Although rapeseed is a first-generation crop, it has gained popularity as a feedstock for biodiesel production due to its high oil content, approximately 40%–45%, and its favorable fatty acid profile [4]. Rapeseed oil (TG) and MeOH form a biphasic system in the reactor, where the reaction occurs at the interface of the two phases, but their immiscibility restricts the mass-transfer rate of reactants to the reaction site.

Poor mixing can result in insufficient contact between the reactants, leading to a slower reaction rate. Efficient mixing is essential to increase the interfacial area between the TG and alcohol phases, thereby minimizing resistance and improving mass-transfer rates [5]. In biodiesel production, the transesterification reaction is often mixed using mechanical stirrers, ultrasonic waves, magnetic stirrers, static mixers, and rotary agitators. Among these, mechanical stirrers and ultrasonic waves are the most commonly used methods for mixing the transesterification reaction in biodiesel production [6, 7]. Mechanical stirring (MS) enhances uniform mixing by increasing the contact surface area between the oil and alcohol phases, thereby improving mass transfer and accelerating the transesterification reaction. However, in viscous systems, it struggles to sufficiently reduce mass-transfer resistance, leading to slower reaction rates. As a result, effective mixing through MS often requires a high-power input, which raises operational costs [8]. Furthermore, achieving uniform mixing at large scale is challenging, often leading to inconsistent product quality and higher production costs. Ultrasound (US), in contrast, improves biodiesel production by generating cavitation and microstreaming, which disrupt boundary layers and intensify mass transfer, leading to faster reaction rates [9]. Beyond its mixing advantages, US is generally more energy-efficient than MS, as localized cavitation reduces both the required mixing time and the amount of catalyst required. Consequently, ultrasound achieves higher biodiesel yields with lower overall energy consumption, making it a promising alternative for sustainable biodiesel production [10].

Production experts and researchers have generated biodiesel experimentally using MS rotation and US frequency. Shahbazi et al. [11] examined 90% biodiesel conversion from RBD (refined, bleached, and deodorized) palm oil, using a 1:6 oil:MeOH molar ratio, 1 wt.% KOH catalysts, and MS rotation of 600 rpm for 60 min under a temperature of 60 °C. According to the study by Lifka et al. [12], the transesterification of canola oil with ethanol has been performed using an ultrasonic probe operating at 24 kHz and 200 W. After 30 min, an 87% conversion was achieved with a 6:1 molar ratio and 0.5%–1% sodium hydroxide. Georgogianni et al. [13] reported achieving an ester yield of nearly 98% using an ultrasonic probe at 24 kHz and 200 W of power from sunflower oil in a mere 40 min. However, MS rotation yielded lower results of about 88%, even after 4 hours

of reaction. A study by Costa-Felixa and Ferreira [14] found that biodiesel production using an 8:1 soybean oil-to-MeOH ratio with a 1% KOH catalyst achieved over 90% conversion in 20 min with ultrasound at 1 MHz without heating, surpassing the 80% conversion obtained by stirring with heating. However, for industrial scalability, mechanical stirring remains the more established and readily implementable option, since conventional stirred-tank reactors are already standard in large-scale biodiesel plants. Ultrasound, while highly efficient at the laboratory and pilot scales, presents challenges for industrial application due to energy dissipation, uneven cavitation distribution in large volumes, and higher equipment costs [6, 7]. Recent advances in continuous-flow ultrasonic reactors indicate promising directions for scale-up, but widespread industrial adoption is still limited compared to mechanical stirring. Hence, a systematic comparison of these two techniques with respect to both energy efficiency and scalability is crucial for guiding future biodiesel process design.

Mathematical models are valuable tools for predicting and optimizing chemical processes [15]. By developing such models for transesterification reactions, biodiesel production can become more cost-effective. These models help optimize reaction parameters and forecast biodiesel yield and quality under various conditions. By applying mathematical modeling and optimal control theory, the production cost can be minimized, while the yield is optimized. Several mathematical model-based studies on base-catalyzed transesterification reactions in biodiesel synthesis have been documented in the literature. Benavides and Diwekar showed the effects of both deterministic control [16] and stochastic control [17] mathematically for biodiesel production in a batch reactor. In 2014, Roy et al. [18] described the effects of stirring profile on limiting mass transfer using mathematical modeling with control theory from *J. curcas* seed oil. Chowdhury et al. [19] showed the effects of temperature and catalyst loading on biodiesel production, and in another study [20] conducted a comparative study of chemical, catalytic, and supercritical methods of biodiesel synthesis. Cao et al. [21] demonstrated the effect of US frequency in reducing mass transfer between TG and MeOH for biodiesel production using mathematical modeling with control from *J. curcas* oil. Despite extensive experimental and theoretical investigations on biodiesel production, several important gaps remain. Most existing studies analyze the effects of mechanical stirring (MS) and ultrasound (US) independently, often emphasizing empirical yield optimization without providing a unified mathematical framework that captures the underlying mass-transfer limitations and their dynamical consequences. In particular, comparative mathematical studies that explicitly quantify how MS and US frequency reduce mass-transfer resistance during transesterification reactions for feedstocks such as rapeseed oil remain scarce. Moreover, the combined use of dynamic modeling, uncertainty quantification, and optimal regulation of mixing intensity has not been sufficiently explored. From a modeling perspective, biodiesel transesterification is inherently governed by interfacial mass transfer between immiscible phases, and variations in mixing intensity directly influence the effective reaction rates. While several studies have employed

optimal control strategies for mechanical stirring or ultrasound frequency separately, a systematic comparison that integrates mass-transfer-based modeling, optimal control theory, and sensitivity analysis within a single framework remains lacking. Additionally, the robustness of biodiesel production models with respect to parametric uncertainty, particularly in reaction kinetics and mass-transfer coefficients, has received limited attention. Beyond biodiesel research, a rapid growth has been observed in the application of advanced computational and mathematical techniques, including optimization, control theory, and data-driven methodologies, for analyzing complex nonlinear systems across diverse scientific and engineering domains [22–24]. These developments highlight the effectiveness of mathematical and computational frameworks in capturing system dynamics, handling uncertainty, and guiding optimal decision-making. Such advances motivate the adoption of rigorous mathematical modeling combined with optimal control strategies in biodiesel process analysis.

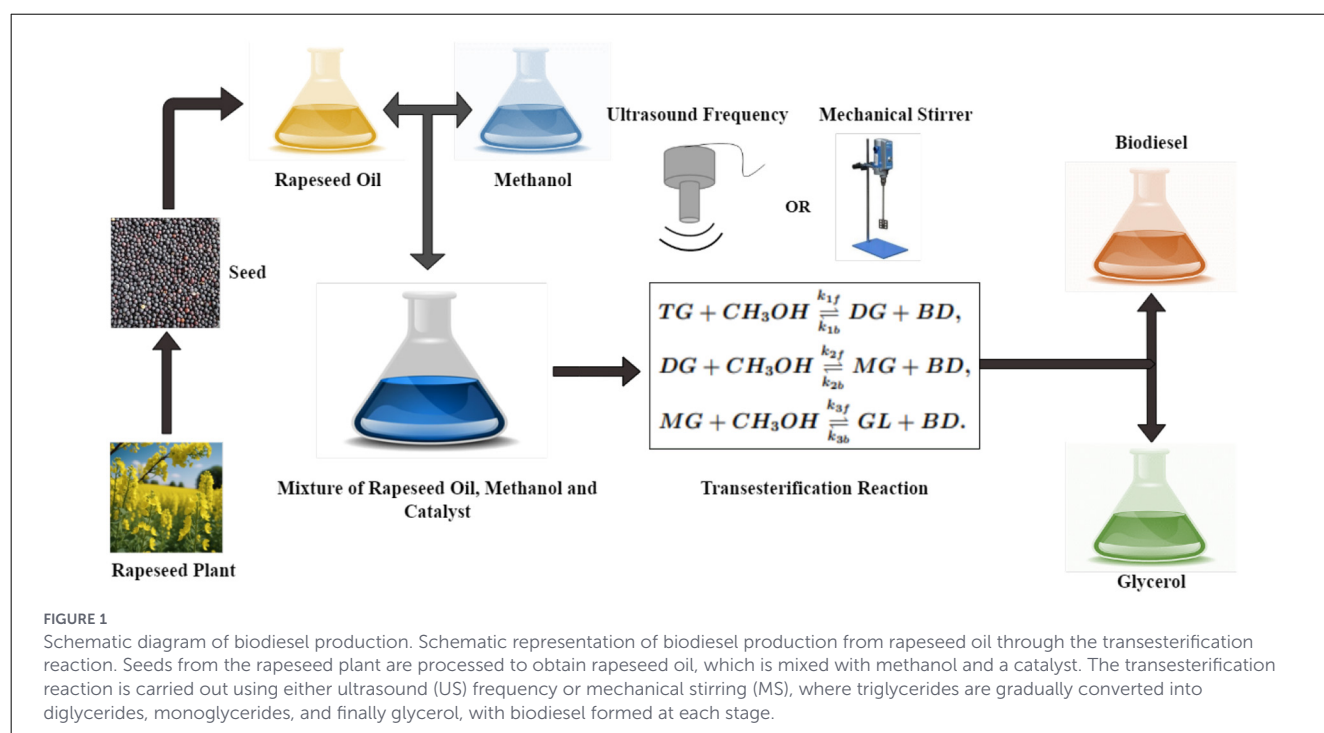
Motivated by these limitations and recent methodological advances, the present study develops a comparative mathematical framework to analyze biodiesel production from rapeseed oil under MS and US frequency. The novelty of this study lies in the combined application of (i) mechanistic mass-transfer-based modeling of MS and US effects, (ii) optimal control theory to regulate stirring speed and US frequency over time in order to efficiently overcome initial mass-transfer resistance, and (iii) uncertainty and sensitivity analysis using the Latin Hypercube Sampling-Partial Rank Correlation Coefficient (LHS-PRCC) approach to identify dominant parameters influencing biodiesel yield. Unlike energy-based assessments, this study focuses explicitly on the role of

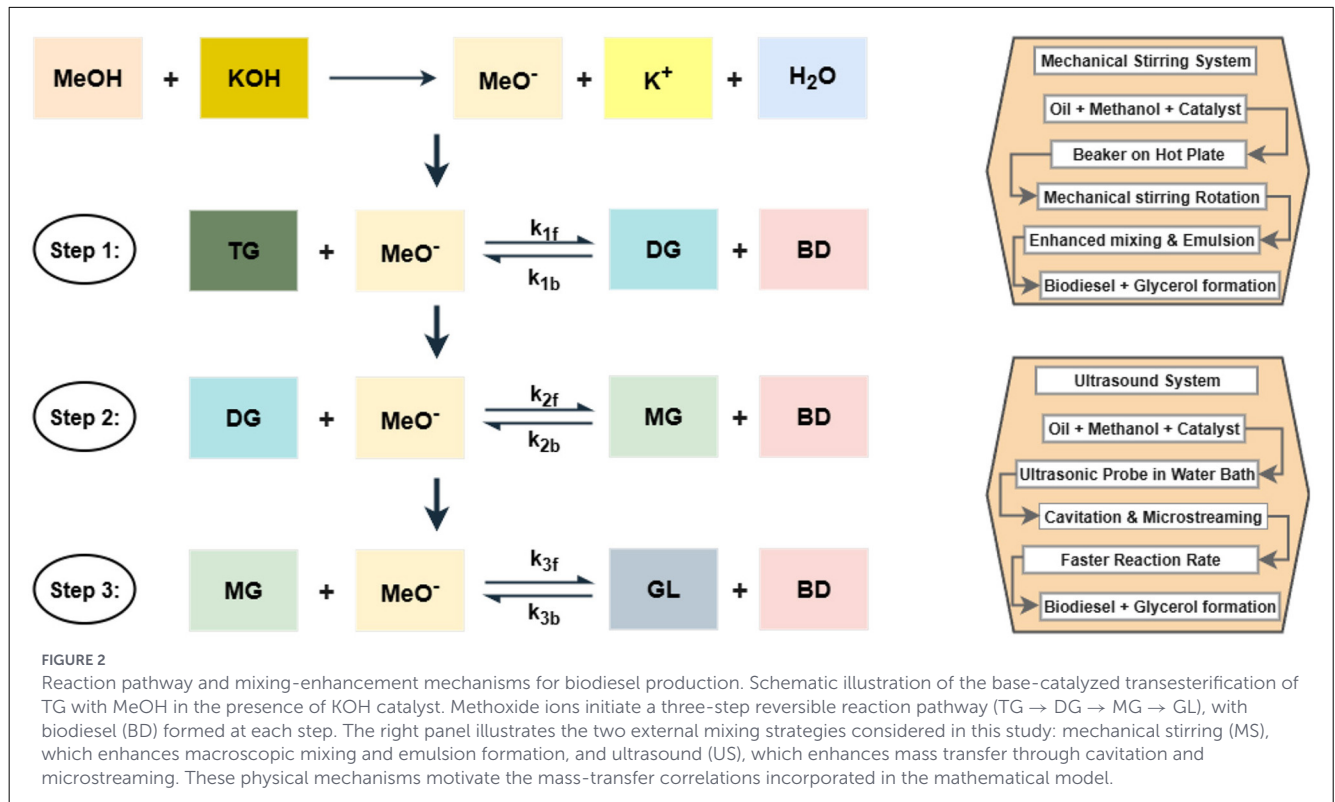
mixing-induced mass-transfer enhancement in governing biodiesel production dynamics.

2 Mathematical model for biodiesel synthesis

In modeling the transesterification reaction between rapeseed oil and methanol (MeOH) for biodiesel production, several assumptions are made to simplify the complex multiphase system:

- (i) The reaction occurs in a liquid-liquid heterogeneous system where triglycerides (TG) and MeOH are immiscible, and mass-transfer resistance is significant during the initial stages of the reaction.
- (ii) Catalyst concentration is assumed constant and uniformly distributed, with no deactivation considered during the reaction period.
- (iii) Physical properties of rapeseed oil (density ρ , viscosity μ , and diffusivity D) are taken as temperature-dependent but spatially uniform within the reactor.
- (iv) The reactor is well-mixed under mechanical stirring (MS) or ultrasound (US) frequency, and temperature is controlled at fixed values (30 °C, 50 °C, and 65 °C).
- (v) Side reactions and soap formation are neglected, and only the three-step reversible transesterification pathway is considered. Schematic diagram of the reaction steps are shown in Figure 1. In Figure 2, the reaction pathway and mixing-enhancement mechanisms for biodiesel production are presented.





2.1 Mass-transfer correlations

To quantify the enhancement of mass transfer under external mixing, two correlations are employed:

Mechanical stirring (MS): mechanical stirring increases the interfacial area between oil and MeOH by generating turbulence and circulating reactants. The empirical correlation used is:

$$K_c = \frac{1}{K_r} = \frac{a}{1 + \exp[-b(f - c)]}, \quad (1)$$

where K_c is the mass-transfer coefficient, K_r is the mass-transfer resistance, f is the agitation speed (rpm), and a , b , c are empirical constants. This sigmoid-type relation is justified because at low stirring speeds, interfacial resistance dominates, while at higher speeds, turbulence reduces resistance and K_c approaches a maximum value [18, 25].

Ultrasound (US) frequency: ultrasound enhances mass transfer by cavitation, bubble collapse, and microstreaming, which disrupt phase boundaries and reduce local viscosity. The modified Dittus-Boelter correlation is applied:

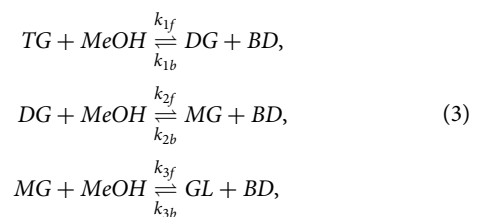
$$M_c = \frac{1}{M_r} = 0.023 \frac{D}{d^2} Re^{0.8} Sc^{0.33}, \quad (2)$$

where M_c is the mass-transfer coefficient, M_r is the resistance, d is the reactor diameter, D is the mass diffusivity of MeOH in oil, ρ is the density of rapeseed oil, μ is the viscosity, and H is the applied ultrasound frequency. The Reynolds number is defined as $Re = \frac{d^2 \rho H}{\mu}$, representing the ratio of inertial to viscous forces, and the Schmidt number is $Sc = \frac{\mu}{\rho D}$, representing the relative thickness

of momentum and mass-transfer boundary layers. This correlation is justified as it captures turbulence and cavitation effects induced by ultrasound [21].

2.2 Reaction scheme

The transesterification of triglycerides (TG) proceeds via three reversible steps:



where DG = diglyceride, MG = monoglyceride, GL = glycerol, and BD = biodiesel. The forward rate constants are k_{1f} , k_{2f} , k_{3f} , and the backward rate constants are k_{1b} , k_{2b} , k_{3b} . Each rate constant follows the Arrhenius relation:

$$k_i = \alpha_i \exp\left(-\frac{E_{\alpha_i}}{RT}\right),$$

where α_i is the frequency factor, E_{α_i} is the activation energy, R is the universal gas constant, and T is the absolute temperature.

2.3 Mathematical model under mechanical stirring

The dynamic concentration profiles of the species are described by:

$$\begin{cases} \frac{dY_A}{dt} = -k_{1f}Y_TY_A + k_{1b}Y_DY_B - k_{2f}Y_DY_A + k_{2b}Y_MY_B \\ -k_{3f}Y_MY_A + k_{3b}Y_GY_B, \\ \frac{dY_T}{dt} = -k_{1f}Y_TY_A + k_{1b}Y_DY_B, \\ \frac{dY_D}{dt} = k_{1f}Y_TY_A - k_{1b}Y_DY_B - k_{2f}Y_DY_A + k_{2b}Y_MY_B, \\ \frac{dY_M}{dt} = k_{2f}Y_DY_A - k_{2b}Y_MY_B - k_{3f}Y_MY_A + k_{3b}Y_GY_B, \\ \frac{dY_B}{dt} = k_{1f}Y_TY_A - k_{1b}Y_DY_B + k_{2f}Y_DY_A - k_{2b}Y_MY_B + k_{3f}Y_MY_A \\ -k_{3b}Y_GY_B + K_cY_B\left(1 - \frac{Y_B}{B_{\max}}\right), \\ \frac{dY_G}{dt} = k_{3f}Y_MY_A - k_{3b}Y_GY_B, \end{cases} \quad (4)$$

where Y_A , Y_T , Y_D , Y_M , Y_B , and Y_G denote the concentrations of MeOH, TG, DG, MG, BD, and GL, respectively. Initial conditions are $Y_A(0) = Y_{A0}$, $Y_T(0) = Y_{T0}$, $Y_D(0) = 0$, $Y_M(0) = 0$, $Y_B(0) = 0$, $Y_G(0) = 0$. The term $K_cY_B(1 - Y_B/B_{\max})$ represents the enhancement of biodiesel production due to MS, where $B_{\max}$ is the maximum achievable biodiesel conversion under ideal (no resistance) conditions.

2.4 Mathematical model under ultrasound frequency

Similarly, to investigate the effect of ultrasound (US) frequency, the mathematical model can be expressed as:

$$\begin{cases} \frac{dY_A}{dt} = -k_{1f}Y_TY_A + k_{1b}Y_DY_B - k_{2f}Y_DY_A + k_{2b}Y_MY_B \\ -k_{3f}Y_MY_A + k_{3b}Y_GY_B, \\ \frac{dY_T}{dt} = -k_{1f}Y_TY_A + k_{1b}Y_DY_B, \\ \frac{dY_D}{dt} = k_{1f}Y_TY_A - k_{1b}Y_DY_B - k_{2f}Y_DY_A + k_{2b}Y_MY_B, \\ \frac{dY_M}{dt} = k_{2f}Y_DY_A - k_{2b}Y_MY_B - k_{3f}Y_MY_A + k_{3b}Y_GY_B, \\ \frac{dY_B}{dt} = k_{1f}Y_TY_A - k_{1b}Y_DY_B + k_{2f}Y_DY_A - k_{2b}Y_MY_B \\ +k_{3f}Y_MY_A - k_{3b}Y_GY_B + M_cY_B\left(1 - \frac{Y_B}{B_{\max}}\right), \\ \frac{dY_G}{dt} = k_{3f}Y_MY_A - k_{3b}Y_GY_B, \end{cases} \quad (5)$$

Here, the effect of ultrasound frequency is represented by the logistic term

$$M_cY_B\left(1 - \frac{Y_B}{B_{\max}}\right),$$

where Y_A = concentration of methanol (MeOH), Y_T = concentration of triglycerides (TG), Y_D = concentration of diglycerides (DG), Y_M = concentration of monoglycerides (MG), Y_B = concentration of biodiesel (BD), Y_G = concentration of glycerol (GL), M_c = mass-transfer coefficient under ultrasound conditions, and $B_{\max}$ = maximum achievable biodiesel conversion in the absence of mass-transfer resistance.

The logistic form is justified because increasing US frequency progressively reduces mass-transfer limitations, but beyond a certain threshold, further increases provide negligible improvement. This captures the saturation effect of ultrasound-enhanced mixing on biodiesel yield.

3 Optimal control problem for maximum biodiesel yield

An optimal control problem involves determining a control policy that will optimize a certain performance criterion for a given dynamic system. This type of problem is prevalent in various fields such as engineering, economics, operations research, and dynamical systems of diseases [26–28]. The optimal control problem is typically represented by a set of differential or difference equations that describe the evolution of the system-state over time [29].

In this study, two mathematical models for biodiesel production have been addressed under some basic assumptions to determine which is more effective among MS and US frequency in maximizing biodiesel yield and minimizing the cost of production. To reduce production costs, we need to regulate or control the MS and US frequency. Here, control $u(t)$ and $z(t)$ are given to the terms K_r and M_r , respectively, to reduce mass-transfer resistance by regulating MS and US frequency over time t .

We want to identify the theoretical optimal ranges for MS and US frequency while keeping the cost function, as measured by time, as low as possible. The ranges of $u(t)$ and $z(t)$ are $0 \leq u(t) \leq 1$ and $0 \leq z(t) \leq 1$, in which $u(t)$ and $z(t)$ represents control input with values normalized between 0 and 1. $u(t)$ or $z(t)$ equal to 1 represents the maximal use of MS or US frequency, and equal to 0 represents no stirring or frequency.

Mathematically, the control-induced system corresponding to the Equation 4 can be formulated as:

$$\begin{cases} F_1 = \frac{dY_A}{dt} = -k_{1f}Y_TY_A + k_{1b}Y_DY_B - k_{2f}Y_DY_A + k_{2b}Y_MY_B \\ -k_{3f}Y_MY_A + k_{3b}Y_GY_B, \\ F_2 = \frac{dY_T}{dt} = -k_{1f}Y_TY_A + k_{1b}Y_DY_B, \\ F_3 = \frac{dY_D}{dt} = k_{1f}Y_TY_A - k_{1b}Y_DY_B - k_{2f}Y_DY_A + k_{2b}Y_MY_B, \\ F_4 = \frac{dY_M}{dt} = k_{2f}Y_DY_A - k_{2b}Y_MY_B - k_{3f}Y_MY_A + k_{3b}Y_GY_B, \\ F_5 = \frac{dY_B}{dt} = k_{1f}Y_TY_A - k_{1b}Y_DY_B + k_{2f}Y_DY_A - k_{2b}Y_MY_B \\ +k_{3f}Y_MY_A - k_{3b}Y_GY_B \\ + \frac{Y_B}{u(t)K_r}\left(1 - \frac{Y_B}{B_{\max}}\right), \\ F_6 = \frac{dY_G}{dt} = k_{3f}Y_MY_A - k_{3b}Y_GY_B, \end{cases} \quad (6)$$

and the control-induced system corresponding to the Equation 5 can be written as:

$$\begin{cases} F'_1 = \frac{dY_A}{dt} = -k_{1f}Y_TY_A + k_{1b}Y_DY_B - k_{2f}Y_DY_A + k_{2b}Y_MY_B \\ -k_{3f}Y_MY_A + k_{3b}Y_GY_B, \\ F'_2 = \frac{dY_T}{dt} = -k_{1f}Y_TY_A + k_{1b}Y_DY_B, \\ F'_3 = \frac{dY_D}{dt} = k_{1f}Y_TY_A - k_{1b}Y_DY_B - k_{2f}Y_DY_A + k_{2b}Y_MY_B, \\ F'_4 = \frac{dY_M}{dt} = k_{2f}Y_DY_A - k_{2b}Y_MY_B - k_{3f}Y_MY_A + k_{3b}Y_GY_B, \\ F'_5 = \frac{dY_B}{dt} = k_{1f}Y_TY_A - k_{1b}Y_DY_B + k_{2f}Y_DY_A - k_{2b}Y_MY_B \\ +k_{3f}Y_MY_A - k_{3b}Y_GY_B \\ + \frac{Y_B}{z(t)M_r}\left(1 - \frac{Y_B}{B_{\max}}\right), \\ F'_6 = \frac{dY_G}{dt} = k_{3f}Y_MY_A - k_{3b}Y_GY_B, \end{cases} \quad (7)$$

with initial conditions for both the Equations 6, 7: $Y_A(0) = Y_{A0}$, $Y_T(0) = 1$, $Y_D(0) = 0$, $Y_M(0) = 0$, $Y_B(0) = 0$, and $Y_G(0) = 0$.

We have formulated the cost function for both Equations 6, 7 as:

$$J[g(t)] = \int_{t_0}^{t_f} [w_1 g^2(t) - w_2 Y_B^2] dt, \quad (8)$$

where $g(t) = u(t), z(t)$. $w_1 (> 0)$ and w_2 are the weight constant on the benefit of the cost function and the penalty multiplier respectively. Since both Equations 6, 7 are of the same type, we will determine the control profile only for Equation 7. Control profile for Equation 6 can be found similarly. Now, we seek to identify the best control $z^*(t)$ such that

$$J(z^*(t)) = \min\{J(z(t)) : z(t) \in Z\},$$

Z is the admissible control set defined by

$$Z = \{z(t) : z(t) \text{ is measurable}, 0 \leq z(t) \leq 1, t \in [t_i, t_f]\}. \quad (9)$$

Now, we employ Pontryagin's Minimum Principle [30] to determine $z^*(t)$.

Theorem 3.1. The control parameter $z^*(t)$ that minimizes $J(z(t))$ over Z are given by $z^*(t) = \max\left(0, \min\left(1, \left\{\frac{\Psi_B Y_B (B_{\max} - Y_B)}{2w_1 M_r B_{\max}}\right\}^{\frac{1}{3}}\right)\right)$, where $\Psi_A, \Psi_T, \Psi_D, \Psi_M, \Psi_B$, and Ψ_G are the adjoint variables satisfying Equations 7 and the following transversality conditions: $\Psi_A(t_f) = \Psi_T(t_f) = \Psi_D(t_f) = \Psi_M(t_f) = \Psi_B(t_f) = \Psi_G(t_f) = 0$.

Proof: The Hamiltonian can be written as:

$$\begin{aligned} \mathcal{H} &= w_1 z^2(t) - w_2 Y_B^2 + \sum_{i=1}^6 \Psi_i F'_i, \\ &= w_1 z^2(t) - w_2 Y_B^2 + \Psi_A (-k_{1f} Y_T Y_A + k_{1b} Y_D Y_B - k_{2f} Y_D Y_A \\ &\quad + k_{2b} Y_M Y_B - k_{3f} Y_M Y_A + k_{3b} Y_G Y_B) + \Psi_T (-k_{1f} Y_T Y_A \\ &\quad + k_{1b} Y_D Y_B) + \Psi_D (k_{1f} Y_T Y_A - k_{1b} Y_D Y_B - k_{2f} Y_D Y_A \\ &\quad + k_{2b} Y_M Y_B) + \Psi_M (k_{2f} Y_D Y_A - k_{2b} Y_M Y_B - k_{3f} Y_M Y_A \\ &\quad + k_{3b} Y_G Y_B) + \Psi_B (k_{1f} Y_T Y_A - k_{1b} Y_D Y_B + k_{2f} Y_D Y_A - k_{2b} Y_M Y_B \\ &\quad + k_{3f} Y_M Y_A - k_{3b} Y_G Y_B + \frac{Y_B}{z(t) \cdot M_r} \left(1 - \frac{Y_B}{B_{\max}}\right)) \\ &\quad + \Psi_G (k_{3f} Y_M Y_A - k_{3b} Y_G Y_B), \end{aligned} \quad (10)$$

where $\Psi_A, \Psi_T, \dots, \Psi_G$ are adjoint variables and $F'_1, F'_2, \dots, F'_6$ are functions defined in Equation 6.

Now, differentiating the Hamiltonian (Equation 10) with respect to $z(t)$ we get:

$$\begin{aligned} \frac{\partial \mathcal{H}}{\partial z^*(t)} &= 0 = 2w_1 z^*(t) - \frac{\Psi_B Y_B (B_{\max} - Y_B)}{M_r B_{\max} z^{*2}}, \\ \implies z^*(t) &= \left\{ \frac{\Psi_B Y_B (B_{\max} - Y_B)}{2w_1 M_r B_{\max}} \right\}^{\frac{1}{3}}. \end{aligned}$$

As $B_{\max} \geq Y_B$ for all values of t , thus $z^*(t)$ will always exist and the value of $z^*(t)$ will be

$$z^*(t) = \begin{cases} 0 & \text{when } \lambda \leq 0, \\ \lambda^{\frac{1}{3}} & \text{when } 0 < \lambda < 1, \\ 1 & \text{when } \lambda \geq 1, \end{cases} \quad (11)$$

where $\lambda = \frac{\Psi_B Y_B (B_{\max} - Y_B)}{2w_1 M_r B_{\max}}$.

Also, by Pontryagin's Minimum Principle, adjoint variables satisfy the following equations:

$$\begin{cases} \frac{d\Psi_A}{dt} = -\frac{\partial \mathcal{H}}{\partial Y_A} &= k_{1f} Y_T (\Psi_A + \Psi_T - \Psi_D - \Psi_B) + k_{2f} Y_D (\Psi_A + \Psi_D - \Psi_M - \Psi_B) \\ &\quad + k_{3f} Y_M (\Psi_A + \Psi_M - \Psi_B - \Psi_G), \\ \frac{d\Psi_T}{dt} = -\frac{\partial \mathcal{H}}{\partial Y_T} &= k_{1f} Y_A (\Psi_A + \Psi_T - \Psi_D - \Psi_B), \\ \frac{d\Psi_D}{dt} = -\frac{\partial \mathcal{H}}{\partial Y_D} &= k_{1b} Y_B (-\Psi_A - \Psi_T + \Psi_D + \Psi_B) + k_{2f} Y_A (\Psi_A + \Psi_D - \Psi_M - \Psi_B), \\ \frac{d\Psi_M}{dt} = -\frac{\partial \mathcal{H}}{\partial Y_M} &= k_{2b} Y_B (-\Psi_A - \Psi_D + \Psi_M + \Psi_B) + k_{3f} Y_A (\Psi_A + \Psi_M - \Psi_B - \Psi_G), \\ \frac{d\Psi_B}{dt} = -\frac{\partial \mathcal{H}}{\partial Y_B} &= 2w_2 Y_B + k_{1b} Y_D (-\Psi_A - \Psi_T + \Psi_D + \Psi_B) \\ &\quad + k_{2b} Y_M (-\Psi_A - \Psi_D + \Psi_M + \Psi_B) + k_{3b} Y_G (-\Psi_A - \Psi_M + \Psi_B + \Psi_G) - \frac{1}{z(t) M_r} \left(1 - \frac{2Y_B}{B_{\max}}\right), \\ \frac{d\Psi_G}{dt} = -\frac{\partial \mathcal{H}}{\partial Y_G} &= k_{3b} Y_B (-\Psi_A - \Psi_M + \Psi_B + \Psi_G), \end{cases} \quad (12)$$

with the transversality conditions $\Psi_A(t_f) = \Psi_T(t_f) = \Psi_D(t_f) = \Psi_M(t_f) = \Psi_B(t_f) = \Psi_G(t_f) = 0$. In a similar way, we can write the control profile for MS, that is, for the Equation 6 as

$$u^*(t) = \begin{cases} 0 & \text{when } \xi \leq 0, \\ \xi^{\frac{1}{3}} & \text{when } 0 < \xi < 1, \\ 1 & \text{when } \xi \geq 1, \end{cases} \quad (13)$$

where $\xi = \frac{\Psi_B Y_B (B_{\max} - Y_B)}{2w_1 K_r B_{\max}}$. $\square$

Remark 3.2. The state Equation 6, costate Equation 12, and the control functions (u^* and z^*) represent the optimal system. Thus, the optimal control problem is a two-point boundary-value problem. We numerically solve the state system forward-iteration method with initial condition, and the costate system using a backward-iteration method with boundary condition $\Psi_i(t_f) = 0$. The control functions are updated in each iteration.

4 Numerical simulation and results

In this section, we have implemented the ode45 solver in MATLAB to numerically visualize the results and understand the chem-dynamical reaction Equations 4, 5). Here, a comparison is made between MS and US frequency to determine the reduction of mass-transfer resistance between MeOH and rapeseed oil (TG) more effectively. The study is performed at three distinct temperatures: 30 °C, 50 °C, and 65 °C, using a vessel with a diameter of 1 m. Biodiesel production is evaluated at each temperature using various MeOH:TG molar ratios, employing both MS and US frequency. Values of parameters are taken from Tables 1, 2 for the simulations.

The molar ratio of MeOH and TG plays a crucial role in the biodiesel production process [31]. Figures 3a–c) shows the comparison of mixing effect using MS and US frequency for biodiesel production at 50 °C in 4:1, 5:1, and 6:1 molar ratios of MeOH and rapeseed oil, respectively. Here, the MS speed is set to 600 rpm, and the US frequency is set to 50 kHz. Figure 3a shows

TABLE 1 Density, viscosity, and diffusivity of rapeseed oil: density, viscosity, and diffusivity of rapeseed oil at three different temperatures.

Temperature °C	Density (ρ) kgm^{-3}	Viscosity (μ) $\text{kgm}^{-1}\text{s}^{-1}$	Diffusivity (D) m^2s^{-1}
30 °C	908.117	97.7575	8.9339×10^{-5}
50 °C	894.735	39.6956	8.7142×10^{-5}
65 °C	881.353	21.9229	8.3704×10^{-5}

The values have been taken from a previous study [46].

TABLE 2 Values of the reaction rate constants: forward and backward reaction rate constants for transesterification reaction using rapeseed oil at three different temperatures taken from a previous study [42].

Rate constant [$\text{L.mol}^{-1}.\text{min}^{-1}$]	30 °C	50 °C	65 °C
k_{1f} (TG $\rightarrow$ DG)	0.0061	0.0359	0.1784
k_{1b} (TG $\leftarrow$ DG)	0.0358	0.1781	0.8134
k_{2f} (DG $\rightarrow$ MG)	0.0767	0.6157	8.2189
k_{2b} (DG $\leftarrow$ MG)	1.3496	6.4165	30.6887
k_{3f} (MG $\rightarrow$ GL)	0.2181	0.4379	0.4717
k_{3b} (MG $\leftarrow$ GL)	0.0013	0.0014	0.0020

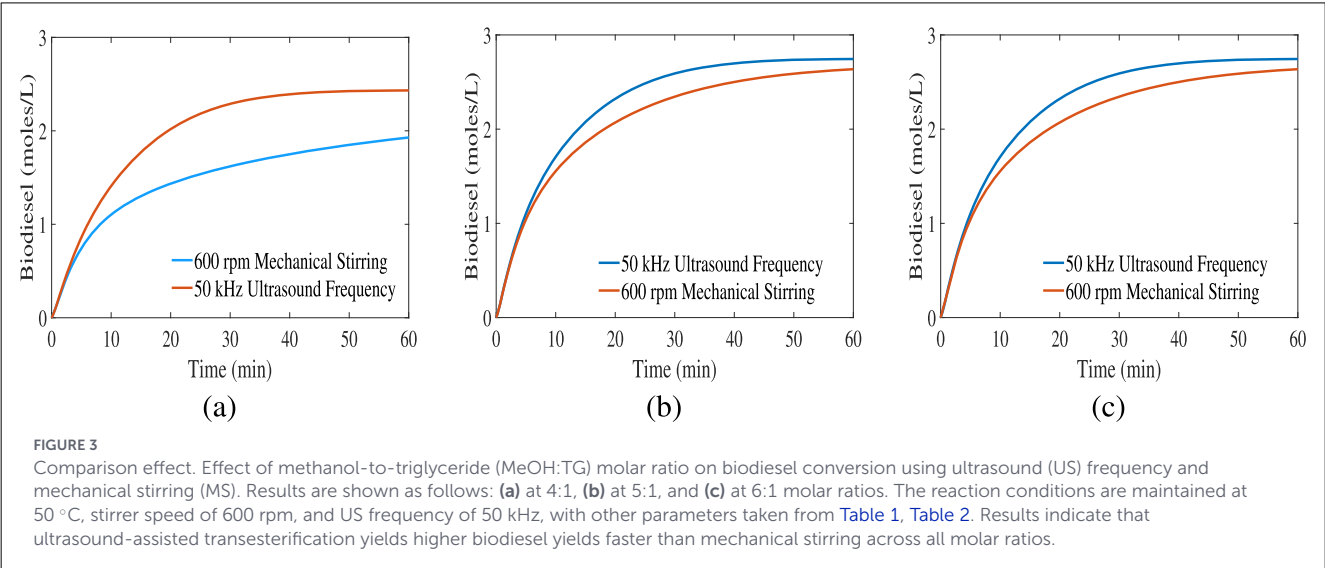
that US frequency reduces the mass-transfer resistance between the reactants more effectively than MS; as a result, higher biodiesel conversion is observed for US frequency. Due to the continuous application of high-intensity MS and US frequency in the system, a certain amount of MeOH evaporates, resulting in an actual MeOH amount below 3 moles and a slight decrease in biodiesel production. From Figures 3b, c, it is clear that US frequency produces more biodiesel compared to MS. The presence of excess MeOH in the system increases the molar conversion of biodiesel for both 5:1 and 6:1 ratios, with the highest production observed at the 6:1 molar ratio. In this way, we have achieved almost 93.66% and almost 95.33% biodiesel yields in just less than 60 and 40 min, respectively,

by the implementation of MS and US frequency, respectively. Hence, the US frequency is more effective than MS at the same molar ratio.

Figure 4 demonstrates how increasing the reaction temperature affects the molar conversion of biodiesel when MS speed, US frequency, and molar ratio of MeOH: TG are maintained at 600 rpm, 50 kHz, and 6:1, respectively. It is evident from these three figures that biodiesel conversion is higher when the US frequency is applied in the system. Figure 4a shows that it takes about 60 min to reduce the mass-transfer resistance between MeOH and oil phases. When the temperature is increased from 30 °C to 50 °C, production increases after 30 min. We have considered the reaction temperature in Figure 4c as 65 °C. At this temperature, biodiesel conversion begins rapidly for both MS and US frequency, but production decreases after 30 min. Due to higher temperatures and continuous high-intensity stirring or high frequency, some MeOH vaporizes, and TG, produced biodiesel, and free fatty acids (FFA) present in the oil react with the catalyst to form soap. This results in lower final production than at 50 °C. This also shows that, for a fixed temperature, US frequency is more effective.

In Figure 5a, the impact of MS on biodiesel production is shown with a MeOH to TG ratio of 6:1 at a reaction temperature of 50 °C. As the stirrer speed increases from 300 to 600 rpm, biodiesel conversion also increases. At 700 rpm, biodiesel production starts rapidly but then decreases after about 25 min, resulting in lower conversion than at 600 rpm. This reduction occurs because higher rotational speeds cause MeOH to vaporize, disrupting the MeOH:oil molar ratio. In Figure 5b, the effect of US frequency is shown for the same molar ratio and temperature. At 50-kHz frequency, we have achieved the highest biodiesel yield. When the frequency is increased to 60 kHz, biodiesel production initially increases, then decreases after about 45 min of reaction. Higher US frequency leads to a slight increase in reaction temperature, causing MeOH vaporization and saponification reactions, which reduce biodiesel yield conversion.

We have performed a global sensitivity and uncertainty analysis using the combined Latin Hypercube Sampling-Partial Rank Correlation Coefficient (LHS-PRCC) framework to assess



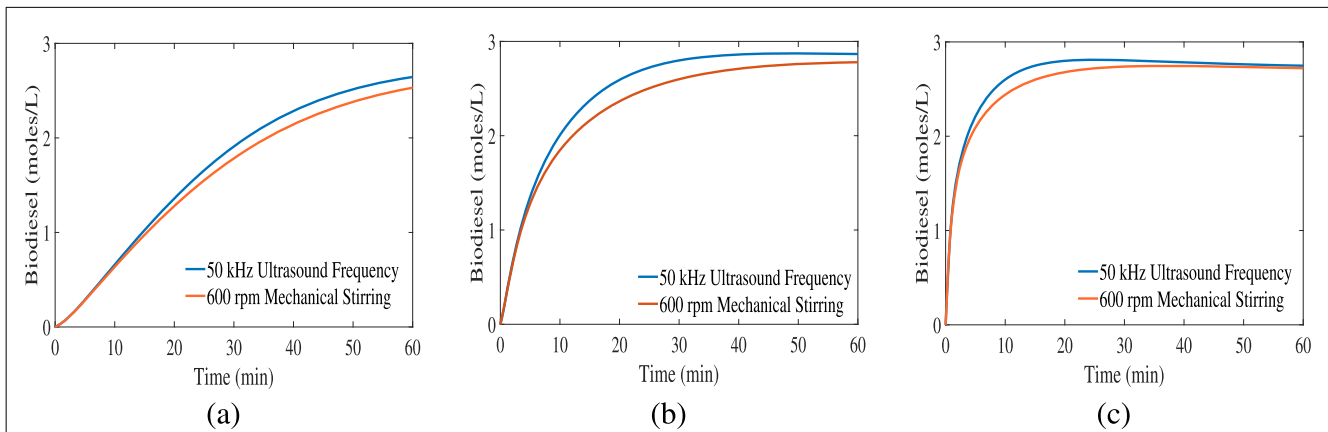


FIGURE 4

Comparison plot: effect of reaction temperature on biodiesel conversion using ultrasound (US) frequency and mechanical stirring (MS). Results are shown as follows: (a) at 30 °C, (b) at 50 °C, and (c) at 65 °C for a MeOH:TG molar ratio of 6:1. The reaction was carried out at MS speed of 600 rpm and US frequency of 50 kHz, with other parameter values taken from Table 1, Table 2. The results demonstrate that higher temperatures enhance the reaction rate, and US-assisted transesterification achieves faster and more efficient biodiesel production compared to MS across all temperatures.

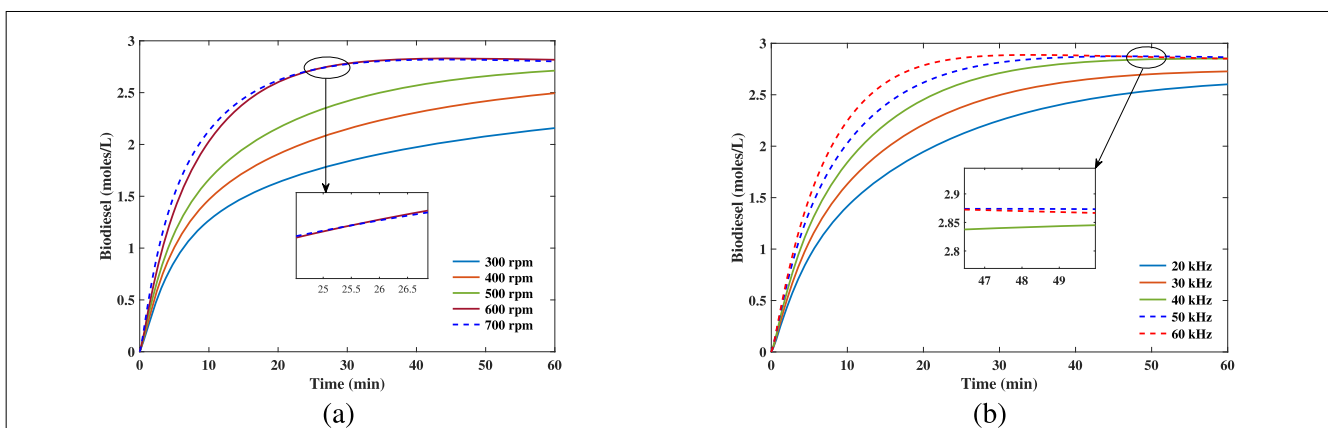


FIGURE 5

MS and US effect: the graph compares the impact of two different mixing methods on the yield of biodiesel from the transesterification reaction. Plot (a) shows the yield achieved across five different speeds of mechanical stirring (MS). Plot (b) shows the yield achieved across five different frequencies of ultrasonic irradiation (US). Here, the MeOH:TG molar ratio is 6:1, and the reaction temperature is 50 °C, with the remaining parameters held constant as per Table 1, Table 2.

the model's robustness to reaction rate constants and mass-transfer coefficients. A total of 1,000 independent random samples have been generated for each model parameter using the Latin Hypercube Sampling (LHS), following uniform probability distributions within their biologically feasible ranges (for methodological details, see the studies by Dutta et al. [32] and Marino et al. [33]). In the bar diagrams (Figure 6), we have demonstrated the sensitivity index of reaction rates and mass-transfer coefficients on final biodiesel yield. This figure allows us to assess the model's robustness to parameter values and identify the parameters that significantly affect the final biodiesel yield. This figure suggests that M_c and k_{2f} are the most positively significant parameters, while k_{1b} and k_{2b} are the most negatively significant parameters for biodiesel production.

To evaluate the statistical relationship between individual parameters and biodiesel yield, scatter plots with corresponding regression lines are shown in Figure 7. These plots illustrate how variations in each reaction rate and mass-transfer coefficient influence the final biodiesel yield across the sampled parameter

ranges. The regression lines represent the best-fit linear trends, providing a qualitative assessment of the direction and strength of the parameter-output relationship. The p-value represents the level of uncertainty associated with each PRCC calculated. For numerical performance, we have considered a preassigned minimum allowed certainty or confidence level of 95% ($p \leq 0.05$) for PRCC values.

Continuous use of high-intensity MS and US frequency causes some MeOH to vaporize from the reaction vessel. As a result, additional methanol must be added to the system to achieve a higher biodiesel yield, thereby increasing production costs. The study aims to maximize biodiesel yield in less time while minimizing production costs. To address these requirements, we have applied optimal control on the MS and US frequency in the system. The system of state Equations 6, 7 coupled with the adjoint Equation 12 has been solved using the forward-backward sweep method (FBSM). In this iterative scheme, the state system is first solved forward in time using an initial guess for the control variables, and the adjoint system is then solved backward in time using the resulting state trajectories. Details of this iterative scheme

have been demonstrated in the Figure 8. The control variables are subsequently updated by applying the optimality conditions until convergence is achieved. These numerical simulations have been performed using MATLAB R2023a, with a sufficiently small time step to ensure solution accuracy and stability.

Figures 9a, b represent the control profile for US frequency and MS, respectively. It is seen from Figure 9a that, initially, a higher

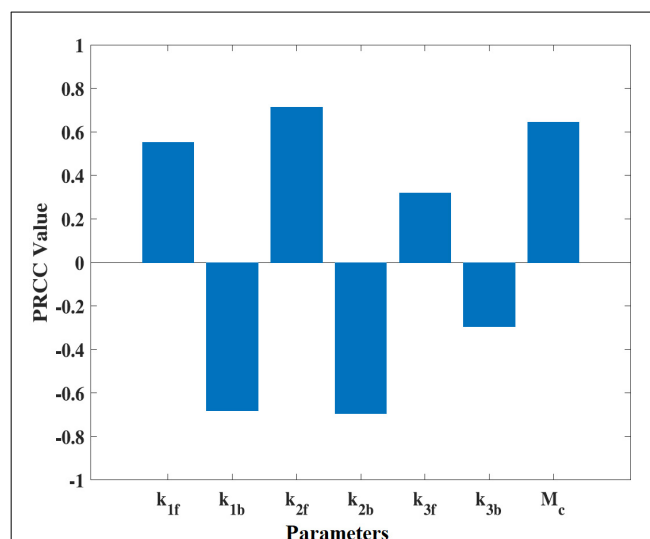


FIGURE 6

Sensitivity index: bar diagram displaying the sensitivity indices of the model parameters with the maximum biodiesel production by Partial Rank Correlation Coefficients (PRCCs) using Pearson's correlation coefficient.

US frequency of 50 kHz is given in the system to reduce the initial mass-transfer resistance between the reactants. After 22 min of reaction, the production has reached its equilibrium, so there is no need to apply further US frequency. We have seen from the above analysis that the US frequency is more effective in reducing the mass transfer limitation than MS (see Figure 6a). It is necessary to give the stirrer a rotation of 600 rpm for a bit longer. After 36 min of reaction, there is no need to increase the rotation, so we can gradually decrease the stirring speed. This phenomenon is plotted in Figure 9b. By regulating the MS and US frequency, MeOH does not vaporize from the system. So, there is always an adequate amount of methanol in the reaction vessel, eliminating the need to add extra methanol to the system. This reduces production costs and enables higher biodiesel production (see Figure 9c). This figure demonstrates that regulating the US frequency for a shorter duration still produces a higher yield compared to MS.

From Figures 3–5, it is observed that the highest biodiesel yield can be achieved at a stirring speed of 600 rpm for MS and at a frequency of 50 kHz for US, individually, when the MeOH:TG molar ratio is 6:1, and the temperature is 50 °C. The bar diagram in Figure 10a illustrates the yield over various reaction times. The diagram clearly indicates that the US frequency is more effective than MS in enhancing mass transfer between the reactants. However, the difference in biodiesel conversion starts to decrease after 30 min. Using the same conditions outlined in Figure 10a, the molar conversion of biodiesel was tracked over time with optimal control methods. Figure 10b visualizes these changes in conversion over time using a bar diagram. The biodiesel yield for these two scenarios, varying temperature, and molar ratio are shown in Table 3. Additionally, comparisons are made for both with and

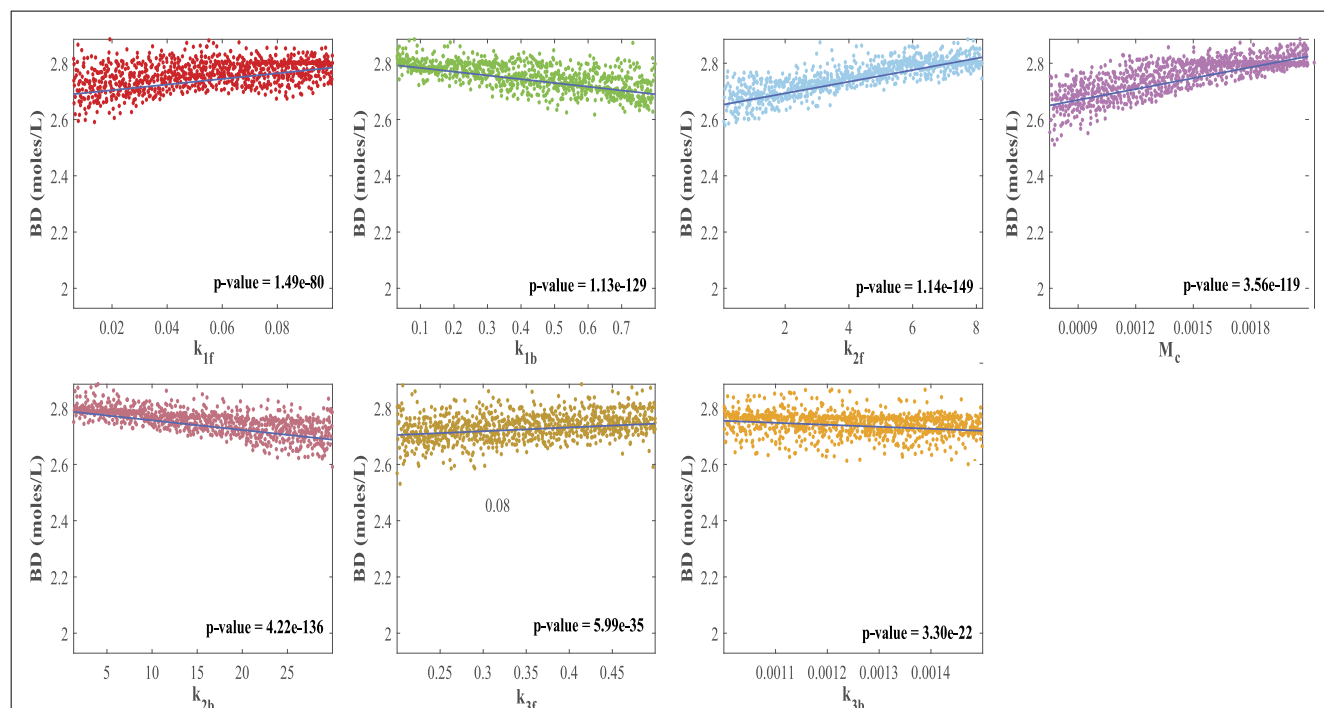


FIGURE 7

Scatter plots: scatter plots represent the different parametric ranges correlated to the biodiesel production with the regression line. Here, the significance level is 0.05, and for each parameter, the sample size is 1,000 based on the LHS approach with a uniform probability distribution.

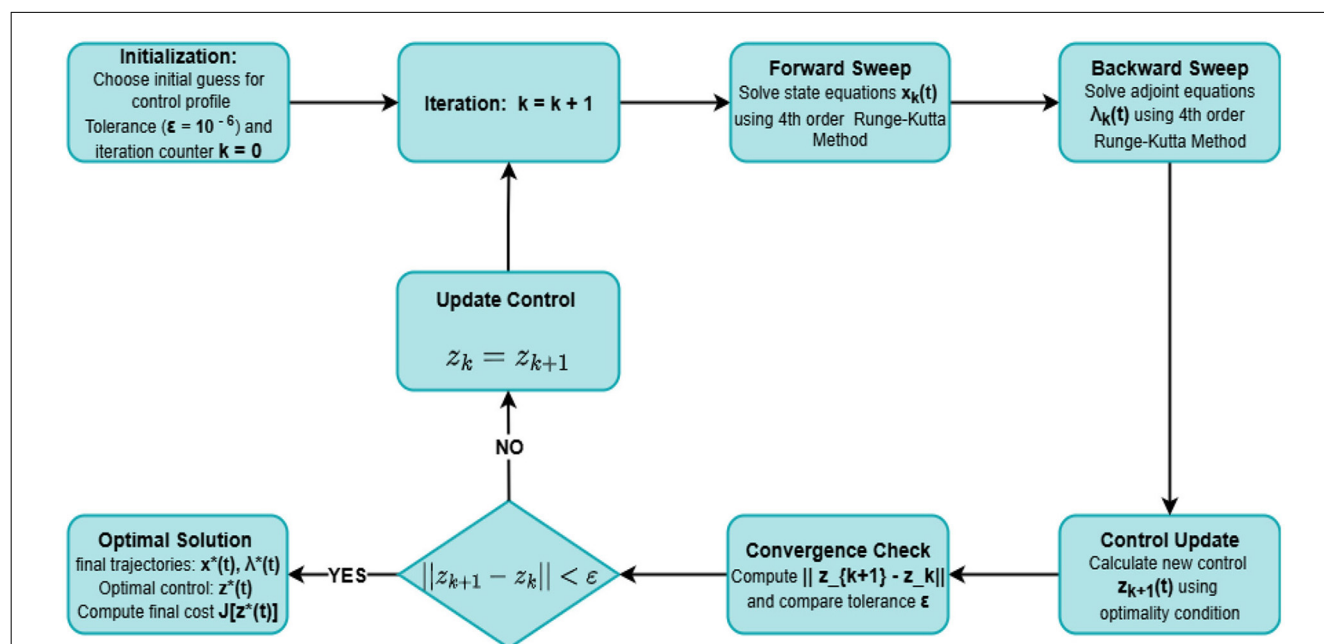


FIGURE 8

Flowchart of the forward-backward sweep algorithm: flowchart of the forward-backward sweep algorithm for numerical solution of optimal control problems. The method solves the two-point boundary-value problem arising from Pontryagin's Minimum Principle through iterative forward integration of state variables and backward integration of costate variables.

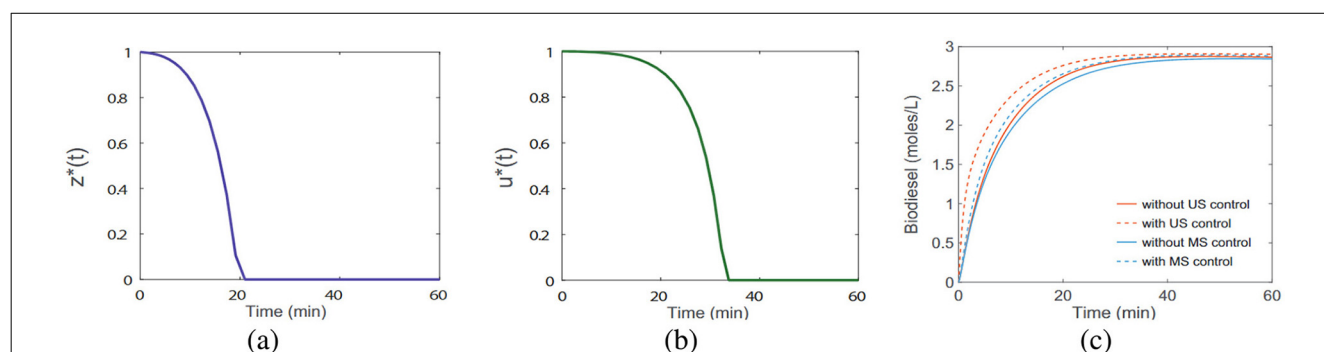


FIGURE 9

Control plot: (a) Control profile for US frequency has been plotted. The reaction was started at 50 kHz US frequency for 22 min; after that, the frequency was reduced. (b) The control profile for MS has been plotted here. MS was maintained at 600 rpm for up to 36 min, after which its speed decreased gradually. In both cases, temperature = 50 °C and MeOH: TG = 6:1, and (c) corresponding biodiesel molar conversion with respect to time and their comparison when no control is applied.

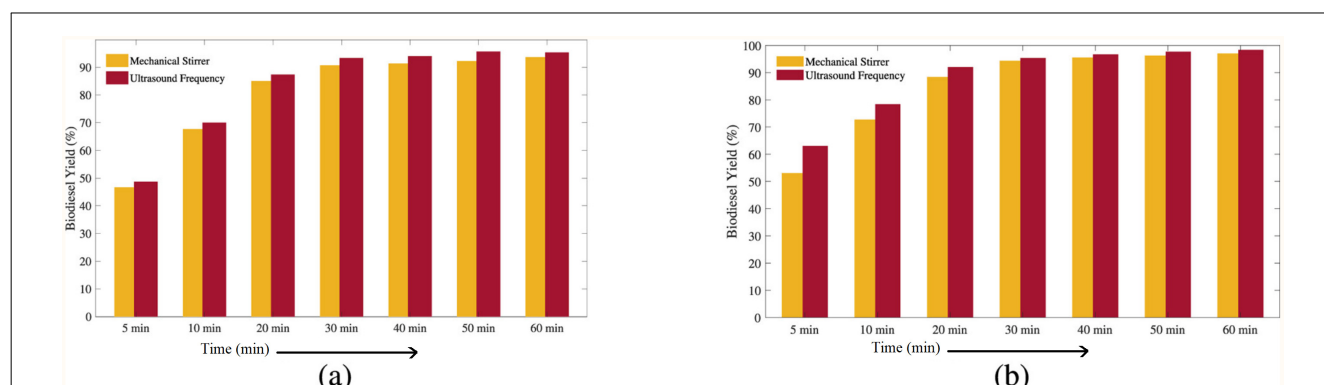


FIGURE 10

Comparison bar diagram: (a) Bar diagram has been plotted to show the biodiesel yield to compare the effectiveness of MS and US frequency without any type of regulation when MeOH: oil = 6:1, temperature is 50 °C, stirrer speed $f = 600$ rpm and US frequency $H = 50$ kHz, (b) Bar diagram has been plotted when we regulate MS and US frequency over time for the same parameter values.

TABLE 3 Summarized numerical results: percentages of biodiesel yields obtained in 20, 40, and 60 min during transesterification reactions at 30 °C, 50 °C, and 65 °C, both with and without optimal control, for different MeOH:oil molar ratios, stirrer speeds, and US frequency, here KOH catalyst concentration is 1 wt%.

Temp. (°C)	Molar ratio (MeOH:TG)	MS rotation (rpm)	US frequency (kHz)	BD yield (%)	BD yield (control) (%)	Reaction time (min)
30	4:1	600	–	54.07	60.00	60
30	4:1	–	50	68.72	74.67	60
30	5:1	600	–	61.30	70.05	60
30	5:1	–	50	71.19	78.67	60
30	6:1	600	–	43.33	61.33	20
30	6:1	600	–	71.66	78.67	40
30	6:1	600	–	84.66	87.33	60
30	6:1	–	50	45.33	63.00	20
30	6:1	–	50	76.00	81.67	40
30	6:1	–	50	81.33	85.33	60
50	4:1	600	–	48.00	57.67	20
50	4:1	600	–	58.00	66.00	40
50	4:1	600	–	64.00	78.67	60
50	4:1	–	50	67.33	75.33	20
50	4:1	–	50	80.00	84.25	40
50	4:1	–	50	81.33	87.67	60
50	5:1	600	–	68.66	75.67	20
50	5:1	600	–	83.33	87.33	40
50	5:1	600	–	88.00	91.67	60
50	5:1	–	50	77.33	83.33	20
50	5:1	–	50	90.00	93.00	40
50	5:1	–	50	91.66	94.33	60
50	6:1	600	–	85.00	88.00	20
50	6:1	600	–	91.33	94.06	40
50	6:1	600	–	93.66	95.32	60
50	6:1	–	50	87.33	95.88	20
50	6:1	–	50	94.00	97.67	40
50	6:1	–	50	95.33	97.00	60
65	6:1	600	–	89.00	94.33	20
65	6:1	600	–	91.33	94.67	40
65	6:1	600	–	90.66	95.33	60
65	6:1	–	50	92.66	96.49	20
65	6:1	–	50	92.33	97.00	40
65	6:1	–	50	91.66	97.67	60

without optimal control, and for MS and US frequency, providing biodiesel yields at 20, 40, and 60 min time intervals. Based on the data provided in Table 3, one can produce 4%–7% more biodiesel yield from rapeseed oil by controlling or regulating MS or US frequency over time in the biodiesel production process, compared to when neither the MS nor the US frequency is controlled.

Once the initial mass-transfer resistance is overcome, the reaction proceeds smoothly. After the initial state of reaction, the intense levels of mechanical stirring (MS) and ultrasound (US) frequency are no longer necessary. Therefore, to make the process

cost-effective and ensure smooth reaction progression, it is essential to control or regulate both MS and US frequency. Here, we have applied optimal control theory to extend our formulated models by incorporating the suitable control parameters (Equations 6, 7). The control inputs $u(t)$ and $z(t)$ are used to regulate the MS and US frequency, respectively, to overcome the initial mass-transfer resistance between MeOH and TG. Evaluated optimal control parameters $u^*(t)$ and $z^*(t)$ (see Equation 11) ensure the optimum use of MS and US frequency for biodiesel production in a cost-effective manner. The numerical representations of optimal control

TABLE 4 Results comparison: the optimal conditions found in the published literature for biodiesel production using various transesterification processes.

Feedstocks	Catalyst	MeOH:TG	Temp. (°C)	MS/US	Time (min)	Outcomes (%) & Methods	References
<i>J. curcas</i> Oil	KOH wt% 1.5	8:1	62	US	15	85.2 (ANN)	[36]
Beniseed oil	Mango, wt% 0.9	6:1	57	MS	60	93.6 (ANN)	[34]
Soybean oil	KOH wt% 1	9:1	60	MS	60	93.2 (ANN)	[47]
Sunflower oil	KOH wt% 0.7	7.5:1	30	US	60	89.9 (ANN)	[37]
Fish oil	KOH wt % 1.55	9.92:1	65	US	32.37	99.2 (RSM)	[39]
<i>J. curcas</i> oil	heteropolyacid wt% 4.23	25:1	65	US	38	96.26 (ANN)	[38]
Palm oil	KOH wt% 2	12:1	50	US	60	92.81 (EXP.)	[35]
Ceiba oil	KOH wt% 1	10:1	60	MS	108	99.80 (ANN)	[40]
Jatropha + Ceiba oil	KOH wt% 0.68	40%v/v	60	MS	120	93.70 (ANN)	[48]
Neem oil	KOH wt% 1.2	7:1	50	US	30	94.47 (RSM)	[49]
<i>J. curcas</i> oil	KOH wt% 1	6:1	50	US	50	97.00 (by controlling US frequency)	[21]
Rapeseed oil	KOH wt% 1	6:1	50	US	40	97.67 (by regulating US frequency)	Present study
Rapeseed oil	KOH wt% 1	6:1	50	MS	60	95.32 (by regulating MS)	Present study

profiles (see Figure 9) demonstrate that initially a higher efficacy of control input [$z^*(t) = 1$ ($H = 50$ kHz)] is required to start the reaction, and after 22 min no further US frequency is needed. In contrast, when we are using MS, a higher efficacy of optimal control parameter [$u^*(t) = 1$ ($f = 600$ rpm)] is required for a longer time (36 min), and then it gradually decreases until the end of the reaction. These results clearly indicate that the US frequency is more suitable for applying as an external effort in an optimal manner to reduce mass-transfer resistance during the reaction.

Through our mathematical study and the application of optimal control theory to MS and US frequency, we have achieved important results while using significantly lower amounts of methanol and catalyst. We have compared our obtained results with the biodiesel production outcomes and optimal conditions reported in previously published articles (see Table 4). Our numerical results showed that, under optimal MS conditions, a 60 min reaction time is required to produce the maximum biodiesel from Rapeseed Oil, while Adepoju et al. [34] reported the same reaction time for producing biodiesel from Beniseed Oil. Sajjadi et al. [35] proposed that 92.81% biodiesel can be extracted from Palm Oil by using MeOH and TG at a ratio 12:1 and US frequency as an external effort. Our simulation results suggest 97.67% biodiesel extraction can be possible from Rapeseed Oil by using MeOH and TG at a ratio 6:1 with optimum US frequency. A large number of experimental and theoretical studies [36–38] suggest that the reaction time can vary within the range 15 – 60 min for different feedstocks while using US frequency as an external effort; these results also satisfy our numerical outcomes, that is, 40 min reaction time is required to produce maximum biodiesel from Rapeseed oil by utilizing optimum US frequency. A few studies also show that more than 99% production of biodiesel is possible from Fish Oil and Ceiba Oil [39, 40], which is a little bit higher than our proposed outcomes. Finally, the present study reports a reaction time of

40 min for US and 60 min for MS (at a fixed temperature of 50 °C), which is notably faster than the reports verified by several other experimental and theoretical studies (see Table 4). This also demonstrates that optimal regulation of US frequency can lead to higher biodiesel production than optimal mechanical stirring. Compared to our previous study using *J. curcas* oil as feedstock [21] under identical reaction conditions, the current study with rapeseed oil demonstrates a higher biodiesel yield achieved in a shorter time when ultrasound frequency is regulated over time in an optimum manner. This highlights the advantage of using rapeseed oil over *J. curcas* oil, though *J. curcas* is a second-generation crop.

The catalyst concentration used for biodiesel production also influences production [41]. To avoid the mathematical complexity, we have used KOH catalyst with a fixed 1 wt% concentration. The study could be improved by capturing the catalyst’s impact in another form. The reaction rates used in this model have been derived from a small experimental study [42], which may not be directly applicable to industrial-scale biodiesel production. Although there are a few limitations, this model study will be highly beneficial for experimental researchers, and they can utilize its optimization techniques for biodiesel production. Our findings can also be extended by incorporating new computational methodologies such as deep learning and transfer learning [43], chaotic system classification [44], and advanced machine learning methods [45].

5 Discussion and conclusion

In this study, we formulated and compared two mathematical models for mechanical stirring (MS) and ultrasound (US) frequency to analyze biodiesel production from rapeseed oil

via transesterification. Based on correlations for mass transfer and application of optimal control theory concepts, the study emphasizes the effects of external mixing operation on conversion efficiency and reaction time. It is clear from the study that after overcoming the initial mass-transfer resistance, there is no need for continuous high-intensity in either MS or US to be used economically through appropriate control.

Numerical simulation results show that US frequency is more efficient than MS in overcoming mass-transfer limitations and yields higher biodiesel yields in shorter reaction times. At 50°C and a methanol-to-oil ratio of 6:1, biodiesel yields of 97.67% in 40 min by US frequency were possible, in contrast to 95.33% in 60 min by MS, under optimal US frequency control. The results agree well with experimentally reported values, confirming that the model predictions are valid across different reaction conditions, as stated by the authors, and paving the way for its further applications in process optimization.

In conclusion, this model can help with reactor design, as it shows that controlled US can reduce methanol and catalyst requirements. In this respect, this model can help develop reactors that use adaptive mixing designs to produce biodiesel. Perhaps future development can include more detailed modeling of catalyst dynamics and viscosity, or computational models, to make it more industrially applicable.

The current study contains some limitations. The model does not account for catalyst deactivation, which could affect long-term predictive capability, or for methanol evaporation, which could introduce variability in controlling concentration or reaction rate. The model will have limited usability when viscosity varies dynamically, which could be due to changes in temperature, concentration, or phase. The model could be expanded to multiphase systems and implemented using integrated computational methods, such as machine learning techniques, to improve its use in the design of biodiesel reactors at a commercial scale.

Data availability statement

The original contributions presented in the study are included in the article/supplementary material, further inquiries can be directed to the corresponding authors.

Author contributions

SA: Conceptualization, Writing – original draft, Formal analysis, Methodology. AR: Formal analysis, Methodology, Writing – original draft. X-ZL: Conceptualization, Methodology, Writing – review & editing. FB: Conceptualization, Supervision, Writing – original draft. PR: Conceptualization, Supervision, Writing – original draft.

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