

## Performance Assessment of Metaheuristic Algorithms: Firefly, Grey Wolf, and Moth Flame in Coal Pyrolysis Kinetic Parameter Estimation

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### Abstract

This study investigates the effectiveness of the Firefly Optimizer (FFA), Grey Wolf Optimizer (GWO), and Moth Flame Optimizer (MFO) metaheuristic algorithms in estimating the kinetic parameters of a single-step coal pyrolysis model. By examining the effects of the algorithmic configuration, the initial parameter estimates, and the search space size on the efficacy and efficiency of the optimization run, the research seeks to encourage the qualified engineering application of these algorithms in the field of pyrolysis modeling. Four critical analyses were conducted: convergence efficiency, robustness and repeatability, parameter tuning, and performance on noisy data. MFO and GWO had comparable fitness scores of  $1.05 \times 10^{-4}$  and  $1.04 \times 10^{-4}$  respectively in the optimisation run analysis, while FireFly Algorithm (FFA) fell behind with a score of  $1.09 \times 10^{-4}$ . Regarding the calculation time, FFA showed better results than other optimizers with an execution time of 113.75 seconds. MFO showed initial promise in convergence analysis with speedy convergence, whereas GWO progressively enhanced its solutions. Additionally, GWO was shown to be the most dependable algorithm with the lowest values for average fitness score and execution time at  $1.07 \times 10^{-4}$  and 38.86 seconds. The combined values of standard deviation in fitness value and execution time for GWO were  $1.07 \times 10^{-6}$  and 0.35 indicating its robustness towards initial parameters. Similar to this, investigations on repeatability emphasized the reliability of the GWO method. Further, the parameter tuning assessments supported the balanced performance of GWO, and the studies of noise handling discovered GWO to be the most robust to noisy data. Overall, GWO is recommended as a one-stop average solution for the general engineered application; however, algorithm choice hinges on the specific requirement.

**Keywords-** Parameter extraction, Metaheuristic algorithm, FFA, GWO, MFO, Coal pyrolysis.

### 1. Introduction

Pyrolysis is an essential aspect of the thermal conversion process (Sakthivel et al., 2023; Stauffer et al., 2008). The majority of conventional methods for producing energy from solids like coal involve a step called pyrolysis (Khare et al., 2011). Thus, coal pyrolysis-a complex process in which heat is used to break down chemicals-has long been a focal point of research in the field of energy science (Li et al., 2015; Lu et al., 2013; Song et al., 2016, 2017; Wang et al., 2012; Yan et al., 2020). This decomposition carried out in an inert environment, makes it possible for coal to be converted into various valuable derivatives, most

notably gas, tar, and char. The by-products highlight the importance of coal pyrolysis in current research with their many uses ranging from energy production to complex chemical synthesis (Schobert & Song, 2002). Central to this process is the kinetics of coal pyrolysis, particularly emphasizing the meticulous evaluation of kinetic parameters. The precision in ascertaining these parameters holds profound implications, influencing not only the efficiency and yield but also the overarching economic viability of coal conversion processes. The design and operating efficiency of pyrolysis reactors are directly impacted by an understanding of the kinetic parameters of coal pyrolysis, including activation energy, frequency factor, and reaction order. These factors are crucial for a wide range of practical applications. For instance, these parameters define the precise temperature and duration of residence required in industrial settings to maximise selectivity and yield. Kinetic parameter information is used in energy production to devise combustion processes that maximise power generation efficiency while reducing emissions of pollutants. This helps to produce cleaner combustion technologies such as low-NO<sub>x</sub> burners. Furthermore, precise modelling of these characteristics is essential for customised syngas generation during coal gasification, which maximises the hydrogen-to-carbon-monoxide ratio for application in procedures like Fischer-Tropsch synthesis. In the production of carbon-based materials, where control over the pyrolysis process affects the structural characteristics of final products like carbon fibres and activated carbon, these factors are just as important (Solomon et al., 1992; Song et al., 2017; van Heek & Hodek, 1994; Yu et al., 2023; Zhang et al., 2010).

The study of pyrolysis attributes and reaction kinetics frequently relies on thermal analysis. Thermal analysis is a method for characterizing materials by tracking the changes in their physical characteristics (primarily weight and energy) when subjected to a controlled temperature treatment. Among the different techniques for thermal analysis, thermogravimetry is a successful and popular technique (Kok & Okandan, 1995; Sauerbrunn & Gill, 1994; Skreiberg et al., 2011; Yang et al., 2007).

Initial insights into pyrolysis modeling were obtained using conventional methods, where the reaction rate is calculated by differentiating or integrating the conversion data (Kök, 2002). Isoconversional models were developed when the intricacy of coal pyrolysis processes became more apparent. Compared to model-fitting techniques, these models, which predict non-isothermal kinetics for the pyrolysis of solid fuels, have proven to be more trustworthy and accurate (Cai et al., 2012; Vyazovkin, 2018). They provided a means of comprehending the kinetics without relying on a specific reaction model. Although TGA offered higher-quality data, more complex techniques were needed to understand it. The complicated reaction processes and non-linear correlations inherent in coal pyrolysis posed difficulties for conventional approaches even after these developments (Dhyani & Bhaskar, 2018). Researchers looked at different strategies, such as meta-heuristic algorithms (Khan et al., 2022; Till et al., 2020). The reaction order, activation energy, and pre-exponential factor are three unknown variables in the Arrhenius degradation equation, which is frequently used to model solid-phase pyrolysis. Numerous estimating techniques have been developed to extract the parameters from the experimental thermal conversion data since they are model-based and not explicitly quantifiable. Curve fitting and optimization have been the most often utilized approaches in recent years. These techniques are particularly effective for multi-reaction complex problems but may take much computational effort.

Over the last two decades, there have been considerable developments in the field of pyrolysis model parameter estimation, which is supported by optimization approaches. Estimating pyrolysis model parameters from experimental data constitutes an inverse problem, where the difficulty resides. This problem is frequently poorly formulated, necessitating strong optimization methods for high-dimensional issues.

The Genetic Algorithm (GA) has traditionally been the key optimization tool in the field of coal pyrolysis modeling (Abdelouahed et al., 2017; Ding et al., 2019; Ferreira et al., 2016; Jain et al., 2016). The Stochastic Hill Climber (SHC) and the Shuffled Complex Evolution (SCE) algorithms became available for pyrolysis parameter estimation as the discipline developed (Ding et al., 2020; Duan et al., 1993). In an extensive study by Lautenberger and Fernandez-Pello, several algorithms, including GA, SHC, SCE, and Genetic Algorithm Simulated Annealing (GASA), were tested for their efficacy in pyrolysis model parameter estimation, with SCE appearing as a superior technique and being advised for a more comprehensive application (Lautenberger & Fernandez-Pello, 2011). Although GA has remained relevant despite criticism and newly developed alternatives, Webster's research claimed that the Stochastic Hill Climber algorithm (SHC) surpassed GA in optimizing the pyrolysis parameters (Webster, 2009).

Meta-heuristic algorithms have become an appealing alternative during the past 20 years (Kumar et al., 2022). These algorithms provide a distinctive solution to optimization issues since they are motivated by natural events and behaviors (Aghbashlo et al., 2019; Ullah et al., 2022; Xu et al., 2017). They are particularly adept at navigating vast solution spaces, avoiding local optima, and finding near-optimal solutions in reasonable time frames (Meng et al., 2021). Pant, Kumar, and Ram used metaheuristic optimization techniques, such as GWO and multi-objective particle swarm (MOPSO), to solve nonlinear equations in various problems, such as hydrocarbon combustion. They showed that their framework can find multiple and better solutions than existing methods (Pant et al., 2019). The authors Uniyal, Pant, and Kumar explored how nature-inspired optimization techniques such as ant colony optimization (ACO), particle swarm optimization (PSO), and grey wolf optimization (GWO) can solve reliability problems. They explained the different types and features of the optimization problems (Uniyal et al., 2020).

The Moth Flame, Firefly, and Grey Wolf Optimisation algorithms were chosen on purpose for this investigation. The moth's celestial navigation inspired the Moth Flame Optimization algorithm, which balances exploration and exploitation to guarantee a thorough search for the ideal solution in the enormous range of kinetic parameter combinations. The Firefly Algorithm, which takes inspiration from the cooperative behavior of fireflies, offers flexibility, a critical quality while negotiating the shifting terrain of options in kinetic parameter estimation. Lastly, the Grey Wolf Optimizer guarantees a systematic and strategic approach to optimization, crucial for the precision required in kinetic parameter estimates by mimicking the leadership hierarchy and hunting mechanism of grey wolves (Kumar et al., 2017, 2019; Mirjalili, 2015; Mirjalili et al., 2014; Negi et al., 2021; Yang, 2009).

These algorithms have been applied in a variety of settings, but more research is still needed to determine how well they work in coal pyrolysis. Preliminary findings indicate potential, but more investigation is needed to determine their efficacy in this context.

This study seeks to offer a thorough assessment of the effectiveness of MFO, FA, and GWO in assessing kinetic parameters of coal pyrolysis, building on the groundwork established by earlier studies. We hope to shed light on these algorithms' effectiveness, robustness, repeatability, and adaptability through rigorous research. We aim to comprehensively understand their potential and restrictions in the context of coal pyrolysis by introducing noise to data, examining algorithm complexity, and modifying the parameters. The study aims to promote the qualified use of these metaheuristic algorithms in pyrolysis modeling by testing their initial values, search space sizes, and overall algorithm settings on the effectiveness of the optimization.

This comparative analysis of metaheuristic algorithms—Firefly Optimizer (FFA), Grey Wolf Optimizer (GWO), and Moth Flame Optimizer (MFO)—serves the practical application of identifying the most

effective method for estimating kinetic parameters in coal pyrolysis. Such a comparison is essential because it makes it possible to choose an algorithm that guarantees precision, computational efficiency, and adaptability under a variety of operating conditions. As an indirect result of this study, the pyrolysis process is optimised, which may result in increased energy efficiency, lower emissions, and financial savings. Understanding the advantages and disadvantages of each algorithm also enables a customised approach to process optimisation, which is essential for sectors looking to maximise output while reducing their environmental effect.

## 2. Optimization

### 2.1 Moth Flame Optimization Algorithm

The celestial navigation of moths serves as the basis for Moth Flame Optimisation (MFO). Moths use celestial cues, primarily the moon, to navigate during their nocturnal forays. The algorithm operates by taking into account a population of moths that are represented by the  $X$  matrix.  $D$  stands for the solution vector's dimensionality, which a moth depicts. The Flame matrix, denoted by the letter  $F$ , is another matrix of moths that the method employs. The Flame matrix represents the ideal solutions up to this point.

To converge to ideal solutions, the algorithm adopts the use of moths' spiraling movement towards flames. The flying behavior of moths makes it seem as if they converge on a flame, and this behavior is used to design the algorithm.

Emulating this, the MFO algorithm captures the spiral movement of moths towards light sources. Mathematically, the distance of the moth from the light source at a given time is represented by the following equations, Equations (1)-(3):

$$D_t = |F_{\text{best}} - X_i| \quad (1)$$

The spiral function,  $S_t$ , is then defined as

$$S_t = D_t * e^{b \cdot l} * \cos(2\pi l) \quad (2)$$

Consequently, the position of the moth in the subsequent time step is given by

$$X_{t+1} = F_{\text{best}} - S_t \quad (3)$$

where,

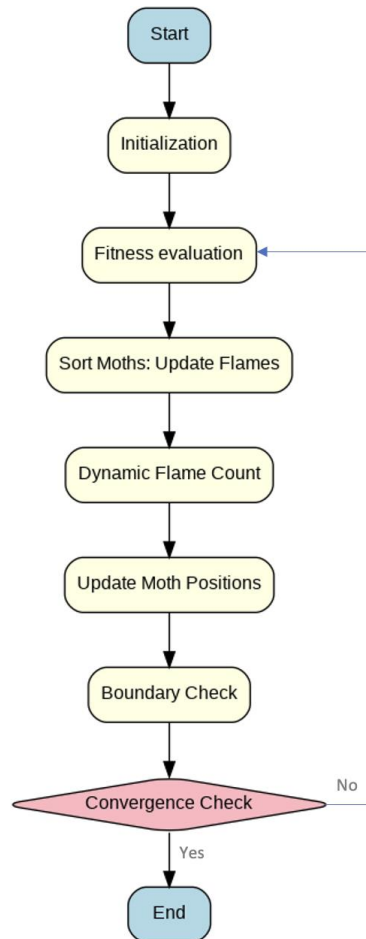
- $D_t$  is the distance of the moth from the light source at time  $t$ .
- $F_{\text{best}}$  is the position of the best solution (brightest light source).
- $X_i$  is the position of the moth.
- $S_t$  is the spiral function, with  $e$  being the base of natural logarithms,  $b$  being a constant, and  $l$  being a random number in  $[-1,1]$ .
- $X_{t+1}$  is the position of the moth at the next time step.

This mathematical representation ensures a balance between exploration and exploitation, making MFO a preferred choice for diverse optimization challenges.

#### **Algorithm Implementation**

The algorithm starts by randomly initializing all the moths' positions within the lower bounds ( $lb$ ), and upper bounds ( $ub$ ), using a uniform distribution. In each iteration  $t$ , the number of flames is dynamically calculated. Each moth's fitness is evaluated using the objective function. The moths are sorted by their fitness values, and the best flames are updated. The distance  $D_t$  between each moth and the flames is calculated. Each moth's position is updated based on this distance and a random component, following an

attractiveness model. The best fitness value achieved in each iteration is stored in a variable. The algorithm terminates after reaching the maximum number of iterations or after meeting convergence criteria. The flowchart of the algorithm is shown in Figure 1.



**Figure 1.** Flowchart of the moth flame algorithm.

## 2.2 Firefly Algorithm

The Firefly Algorithm (FFA) is rooted in the bioluminescent communication behavior of fireflies. Fireflies emit light of varying intensities to attract potential mates. In the algorithm, the attractiveness of a firefly is determined by its brightness, which diminishes as its distance from other fireflies increases. The attractiveness of a firefly is determined by its brightness, which decreases as its distance from other fireflies increases. The brightness or the attractiveness can be represented as Equation (4):

$$\beta(r) = \beta_0 * e^{-\gamma r^2} \quad (4)$$

where,

- $\beta_0$  = Attractiveness at  $r = 0$  or initial brightness.
- $\gamma$  is the light absorption coefficient.
- $r$  is the distance between two fireflies.

If a firefly is less bright than another, it will move towards the brighter one. This movement is mathematically represented by considering the initial brightness, light absorption coefficient, and the distance between two fireflies. The movement is given by Equation (5):

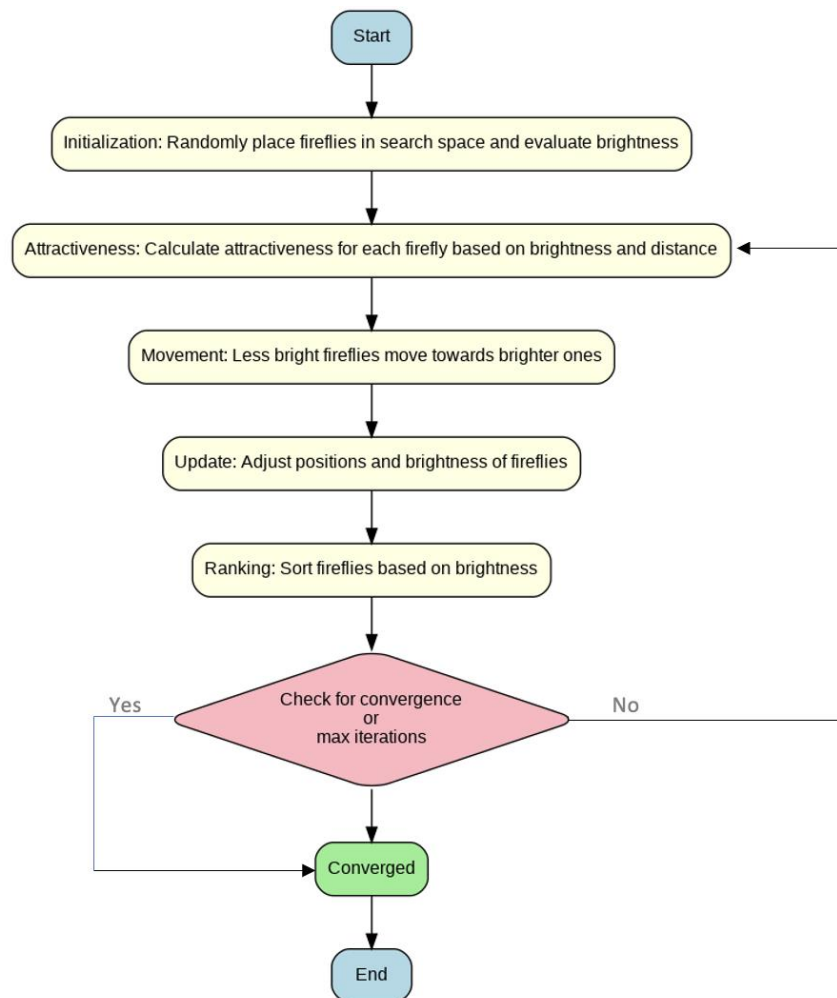
$$x_i = x_i + \beta(r_{ij}) \cdot (x_j - x_i) + \alpha(\text{rand}() - 0.5) \quad (5)$$

where,

- $X_i$  and  $X_j$  are the positions of the two fireflies.
- $r_{ij}$  is the Euclidian distance between fireflies  $i$  and  $j$ .
- $\alpha$  is a randomization parameter.
- $\text{Rand}()$  is a random number in  $[0,1]$ .

The adaptability of the Firefly Algorithm, stemming from its dynamic attractiveness based on brightness, makes it a versatile tool for optimization problems, especially in scenarios with dynamic conditions.

### Algorithm Implementation



**Figure 2.** Flowchart of the firefly algorithm.

The firefly algorithm is initiated by randomly placing a population of fireflies within the search space and evaluating their brightness (fitness) values. Then, each firefly's attractiveness to every other firefly is calculated based on their relative brightness and distance. The dimmer fireflies move towards the brighter ones according to their attractiveness. A random component is introduced into the function defining the movement of the fireflies to ensure thorough exploration of the search space. After the movement, the algorithm updates each firefly's positions and brightness values and sorts them in descending order of their brightness. This process is repeated for a predefined number of iterations or until a convergence criterion is met. The flowchart of the algorithm is given in Figure 2.

### 2.3 Grey Wolf Optimizer Algorithm

Grey Wolf Optimizer (GWO) is inspired by the social hierarchy and hunting mechanism of grey wolves. In the wild, grey wolves exhibit a structured hierarchy, with alphas leading the pack, followed by betas and deltas, while the rest are categorized as omegas. In GWO, this hierarchy is simulated, with the leading three wolves guiding the hunt with alpha as the dominant leader, beta as the subordinate to alpha and assisting in decision making, gamma as the scout and subordinate to alpha and beta, and omega as the followers. The positions of the wolves are updated based on the guidance of the alpha, beta, and delta wolves. GWO's structured and strategic approach to optimization, simulating the hunting behavior of grey wolves, makes it apt for problems demanding precision and thorough exploration.

The mathematical representation of their hunting behavior involves coefficient vectors and the positions of the leading wolves, which guide the rest of the pack. The GWO uses an iterative process to update the positions of the wolves (solutions). The positions of the wolves towards the three dominant wolves are updated using the following equations, Equations (6)-(10):

$$A = 2a * \text{rand}() - a \quad (6)$$

$$C = 2 * \text{rand} \quad (7)$$

$$D_{\text{wolf}} = |C * \text{Position}_{\text{wolf}} - \text{Position}| \quad (8)$$

$$X = \text{Position}_{\text{wolf}} - A * D_{\text{wolf}} \quad (9)$$

where:

- A and C are coefficient vectors.
- a decrease linearly from 2 to 0 over iterations.
- rand is a random vector in [0,1].
- $X_{\text{wolf}}$  is the position of the leading wolf (alpha, beta, or delta).
- $X_i$  is the position of a specific wolf.

The positions of the alpha, beta, and gamma wolves influence the new position of each wolf:

$$\text{New Position} = \frac{(X_{\alpha} + X_{\beta} + X_{\gamma})}{3} \quad (10)$$

#### **Algorithm Implementation**

The first step in the implementation of the algorithm is randomly initializing the positions of the wolves in the search space. This is followed by sorting the wolves based on their fitness values, where the top three wolves are designated alpha, beta, and gamma. Based on this, for each wolf in the population, the position of the wolves with respect to the three dominant wolves is updated using the mathematical model. The fitness value for this newly updated position is evaluated to check if it's a lower value (better solution) if so then the algorithm replaces the current position with the new one. After all the wolves have been updated, their fitness values are re-evaluated and re-sorted. The procedure is repeated for a maximum number of iterations or until convergence criteria are met. The flowchart of the algorithm is given in Figure 3.

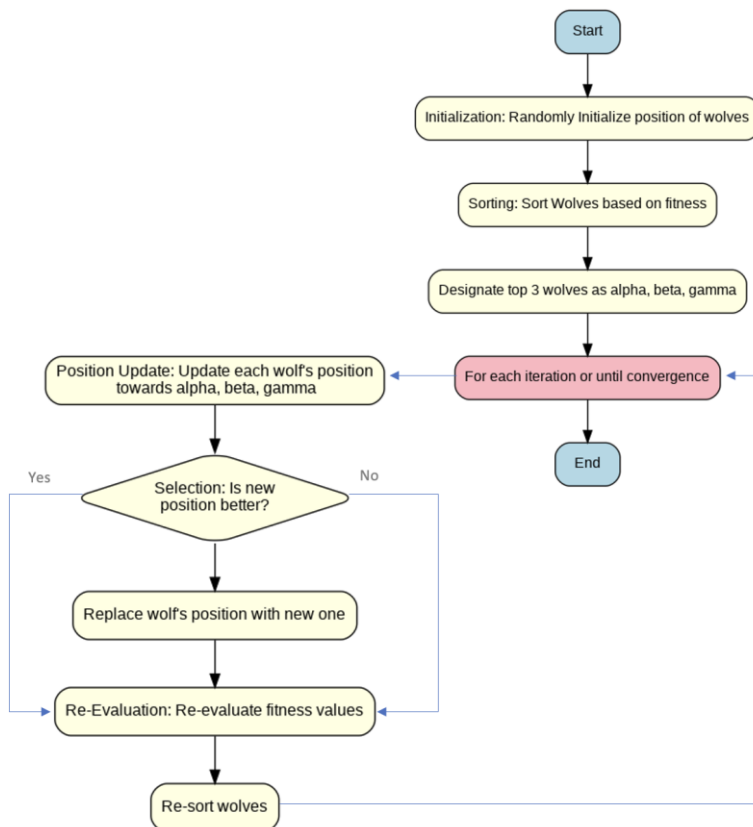


Figure 3. Flowchart of grey wolf optimiser algorithm.

### 3. Experimental Data, Description of The Kinetic Model, and its Mathematical Implementation

#### 3.1 Samples

Coal samples were collected from Singrauli mines in approximately 5 kg. These bulk samples were broken and crushed into smaller pieces before grinding using mortar. The ground powder was then sieved for particle sizes of 0.15 mm. The images of the bulk samples and powdered samples are shown in Figures 4 and 5.



Figure 4. Image of bituminous bulk sample.



Figure 5. Image of powdered bituminous sample.



Non-isothermal TGA data for coal pyrolysis was collected by carrying out TG experiments in an inert nitrogen atmosphere using NETZSCH STA 449 F3 Jupiter equipment for three heating rates, 10, 20, and 30 K/min. The samples were heated from ambient temperature to 1300 °C.

The thermal decomposition is modeled using a single-step reaction model that can be represented as, Equations (11) and (12):

$$\frac{d\alpha}{dt} = kf(\alpha) \quad (11)$$



where, X is the final char mass fraction, and alpha is the conversion mass fraction given by Equation (13):

$$\alpha = \left( \frac{m_0 - m}{m_0 - m_f} \right) \quad (13)$$

where,  $m_0$  is the initial mass of the sample,  $m_f$  is the final mass of the sample, and  $m$  is the mass of the sample at that particular time step. The reaction rate was modelled using the equation, Equation (14):

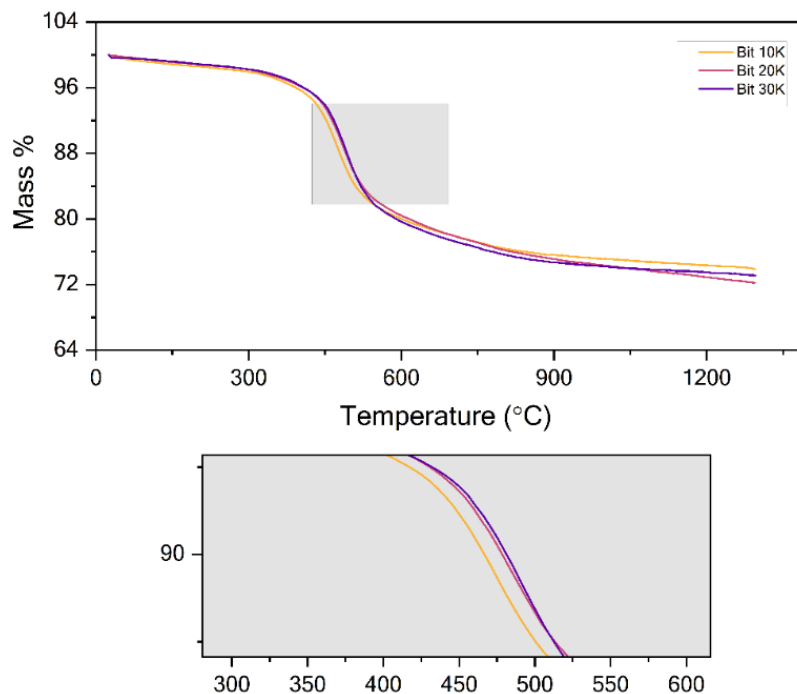
$$\text{reaction\_rate}(T, \alpha, A, E, n, \beta) = \frac{(A * e^{(-E/R * T)}) * (1 - \alpha)^n}{\beta} \quad (14)$$

where, T is the temperature,  $\alpha$  represents conversion, A is the pre-exponential factor, E is the activation energy, n is the reaction order,  $\beta$  is the heating rate, and R is the universal gas constant.

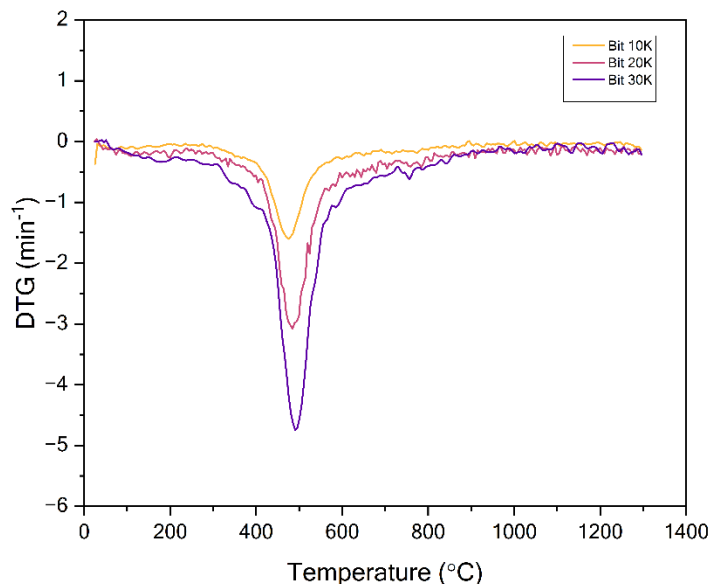
## 4. Results and Discussions

### 4.1 TG Profile

DTG and mass loss profiles of the bituminous coal for the three heating rates are illustrated in Figures 6 and 7.



**Figure 6.** DTG curve of bituminous coal.



**Figure 7.** DTG curve of bituminous coal.

The pyrolysis process may be divided into a threefold system, starting with the desorption phase. Moisture and adsorbed gaseous components are released as temperatures rise during this early phase. This process lasts until temperatures reach around 300 °C. The fast devolatilization phenomenon is then present in the stage that is characterized by a significant decrease in mass. This phenomenon is followed by increased temperature, making it easier for covalent bonds to break. The disintegration of tar precursors, gaseous emission, and semi-coke formation occurs within the heat range of 400–600 °C, after the preliminary phase's breakdown of weak bonds. The gasification of carbonaceous residues, which results in the formation of CH<sub>4</sub>, CO, and H<sub>2</sub> gases, stabilizes the mass loss rate beyond the threshold temperature of 800 °C.

#### 4.2 Optimization Runs

Three different algorithms—the Firefly Algorithm (FFA), the Grey Wolf Optimizer (GWO), and the Moth Flame Optimizer (MFO)—were used to estimate kinetic parameters using TGA data.

In GWO, a small constant EPSILON is added to the denominator of the exponential term for computational stability. The goodness of fit between model predictions and experimental data was quantified using a least-squares objective function, Equation (15):

$$\text{Objective}(\text{parameters}, T, \alpha, \left(\frac{d\alpha}{dT}\right)_{\text{exp}}, \beta) = \Sigma \left( \left( \left(\frac{d\alpha}{dT}\right)_{\text{model}} - \left(\frac{d\alpha}{dT}\right)_{\text{exp}} \right)^2 \right) \quad (15)$$

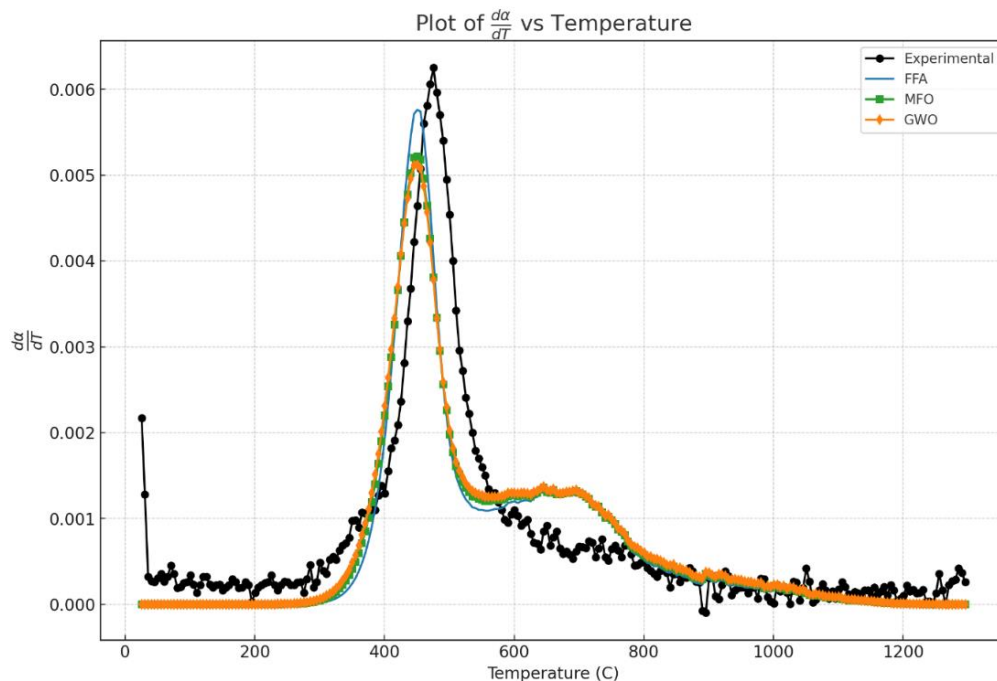
**Improved Model Fitting:** Determining the kinetic parameters through minimizing the objective function is based on comparing the model-predicted rate of change of conversion,  $d\alpha/dT$ , with the experimentally observed rate, which helps improve model accuracy. This is because minor rate discrepancies can lead to significant differences in cumulative values over time. Opting to calibrate the model based on the rate of change ensures a more faithful representation of the underlying process dynamics, which can be more informative than just looking at the extent of reaction or decomposition. Focusing on the rate is equivalent to looking at how rapidly a substance decomposes or reacts at various temperatures, which may be more insightful than only considering the degree of conversion or breakdown.

The best estimates of the kinetic parameters were achieved by iteratively adjusting the parameters of each optimization algorithm to minimize this objective function. To guide the optimization process, certain boundaries were established, such as lower bounds (lb),  $[1e^3, 1e^4, 1]$  and upper bounds (ub)  $[1e^{12}, 2e^5, 6]$  for A,  $E_a$ , and n. These bounds define the search space for the algorithm to work within. Along with the bounds, the maximum number of iterations, 2000, and the number of search agents (Number of Search Agents, NSA: moths, fireflies, wolves), 1000, were held common across the three algorithms. The results from the optimization runs are encapsulated in Table 1, given below.

**Table 1.** Results of the optimized values obtained from the three algorithms.

Algorithm	Pre-exponential factor A (1/min)	Activation energy $E_a$ (J/mol)	Order of reaction n	Best Fitness Value	Execution Time (seconds)
GWO	$2.99 \times 10^8$	$1.30 \times 10^5$	4.6130	0.00010473	159.42
MFO	$2.54 \times 10^9$	$1.42 \times 10^5$	4.9705	0.00010527	113.75
FFA	$3.91 \times 10^8$	$1.31 \times 10^5$	4.6750	0.00010941	404.55

The GWO, MFO, and FFA algorithms prove to be highly effective in fitting data. In particular, MFO obtains a fitness value of 0.00010527, which is practically identical to GWO's 0.00010473, but FFA records a slightly higher value of 0.00010941, indicating a slight inaccuracy. Interesting insights may also be gained from time efficiency, where MFO leads with a computational time of 113.75 seconds, followed by GWO at 159.42 seconds, and finally, FFA at 404.55. This demonstrates that MFO is the best option when time restrictions are crucial. Additionally, parameter examination reveals that MFO has the lowest pre-exponential factor 'A' at  $2.54 \times 10^9$  and the highest activation energy ' $E_a$ ' at  $1.42 \times 10^5$ . Slight variation in reaction order 'n' is found across all algorithms, with MFO showing the highest value of 4.9705, while the highest pre-exponential factor found is for FFA. The comparison of the conversion rate predicted by each algorithm is visualized in Figure 8.



**Figure 8.** Rate change of alpha vs. Temperature as predicted by each algorithm.

In conclusion, the data indicates that all three methods can accurately calculate the kinetic parameters of coal pyrolysis. Significant variations in fitness levels and other factors are not observed to distinguish one algorithm as being better than the other. The choice between them would likely hinge on external factors such as computational time or other problem-specific constraints and requirements.

### 4.3 Convergence Analysis

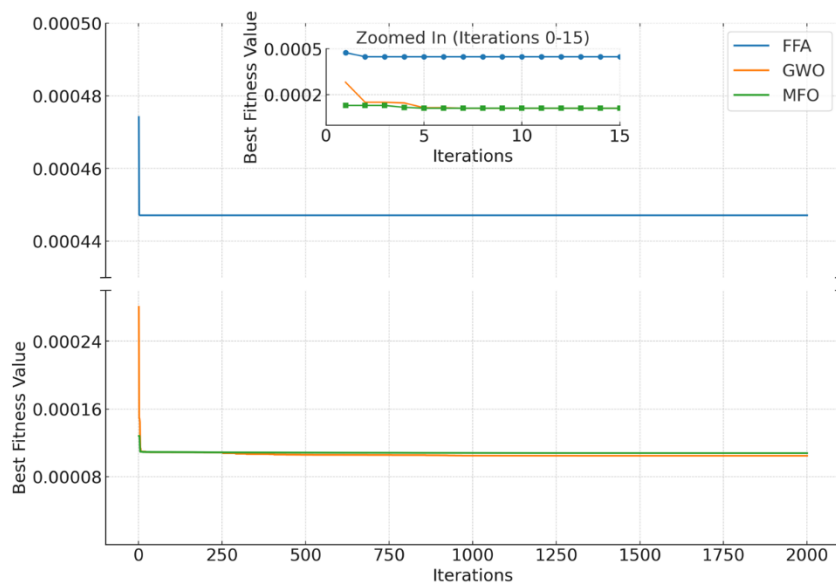
The objective was to evaluate the speed and consistency with which each metaheuristic algorithm—the Firefly Algorithm (FFA), the Grey Wolf Optimizer (GWO), and the Moth-Flame Optimizer (MFO)—approached the optimal solution in the estimate of kinetic parameters. Each method's fitness value across several iterations was tracked to gauge convergence. The following were considered:

- (i) Initial Fitness Value: The starting fitness value at the first iteration.
- (ii) Final Fitness Value: The fitness value at the last recorded iteration.
- (iii) Convergence Rate: The rate at which the fitness value approaches the optimal solution.

The results from the convergence analysis are listed in the Table 2 given below and Figure 9 shows the Visual representation of the convergence pathways of each algorithm.

**Table 2.** Results from the convergence analysis.

Algorithm	Initial Fitness Value	Final Fitness Value	Convergence Rate
FFA	0.000474	0.000447	-0.057
GWO	0.000280	0.000105	-0.625
MFO	0.000128	0.000108	-0.156



**Figure 9.** Visual representation of the convergence pathways of each algorithm.

It is evident from Figure 9 that MFO stands out as the most promising algorithm in terms of initial fitness values since it begins closer to the ideal outcome. In Figure 9, MFO (green line) begins with the smallest fitness values of the three algorithms and finishes above GWO (orange line), implying that the convergence rate is slower than GWO. Even from the figure, the slope of the curves is distinguishable with MFO displaying the highest slope, implying the highest convergence rate. GWO shows a notable ability to

improve its solutions as the iterations go on despite starting with a greater fitness value. Even though it is reliable, the FFA doesn't show the same level of quick convergence as the other two. The MFO curve is relatively constant when the convergence rate is observed, indicating that it may have discovered an area around the global optimum very quickly even in the initial stages of the optimization process. GWO, on the other hand, exhibits a more dynamic search and continuously improves its solutions. FFA's stable state and smaller slope value show that it actively seeks the best answer, although more slowly.

A more thorough examination using longer iterations and different beginning circumstances might give greater insight into the algorithms' performances, considering the ultimate fitness values. However, based on this data, MFO appears to provide the optimal compromise between the quality of the initial solution and convergence stability.

#### 4.4 Robustness Testing

The Robustness Analysis's primary goal is to evaluate the stability and dependability of the three metaheuristic algorithms Firefly Algorithm (FFA), Grey Wolf Optimizer (GWO), and Moth-Flame Optimizer (MFO) under different initial conditions or settings. To prove its dependability for the task of predicting kinetic parameters, a resilient algorithm should retain a high degree of performance despite these modifications. Random initialization is done within a given range for each kinetic parameter  $A$ ,  $E_a$ , and  $n$ . A broad range based on literature data and empirical understanding of the coal pyrolysis process was defined in order to choose the bounds for the initial value estimates for the kinetic parameters ( $A$ ,  $E_a$  and  $n$ ). The goal of this strategy was to guarantee that the search space was adequately investigated without limiting the optimizers to a small area that would skew the outcomes.

The robustness study was aimed at evaluating the impact of these initial parameters on the optimisation results. In this investigation, each optimisation algorithm (FFA, GWO, and MFO) was run 10 times, with initial parameters generated at random within the specified common ranges. Using a multiple-run approach, the consistency and dependability of the optimisation outcomes were assessed in relation to the variation in initial positions. The results from this analysis are tabulated in Table 3 given below. The analysis, which is presented in Tables 3 and 4, shows that the optimisation algorithms continuously converged to similar solutions even when the initial values were randomly chosen.

**Table 3.** Kinetic parameters estimated in the robustness analysis.

Algorithm	Avg. $A$	Std. Dev. $A$	Avg. $E_a$	Std. Dev. $E_a$	Avg. $n$	Std. Dev. $n$
FFA	$4.32 \times 10^{11}$	$3.27 \times 10^{11}$	$16.8 \times 10^4$	$5.04 \times 10^3$	5.71	0.159
GWO	$2.18 \times 10^{11}$	$2.72 \times 10^{11}$	$15.3 \times 10^4$	$18.7 \times 10^3$	5.29	0.545
MFO	$4.74 \times 10^{11}$	$3.47 \times 10^{11}$	$15.7 \times 10^4$	$91.8 \times 10^3$	3.03	1.500

**Table 4.** Key statistics from the robustness analysis.

Algorithm	Avg. Fitness	Std. Dev. Fitness	Avg. Execution Time (Seconds)	Std. Dev. Execution Time
FFA	$1.28 \times 10^{-4}$	$1.78 \times 10^{-5}$	241.29	1.86
GWO	$1.07 \times 10^{-4}$	$1.90 \times 10^{-6}$	38.86	0.35
MFO	$4.08 \times 10^{13}$	$1.29 \times 10^{14}$	8.32	0.61

The average value of the kinetic parameters as well as the fitness values acquired throughout the runs reflects this. The standard deviations of the fitness values show a moderate spread in the range of  $10^{-5}$  and  $10^{-6}$  for FFA and GWO respectively, whereas MFO has a significant value in the range of  $10^{14}$ . This indicates that the optimisation process's accuracy or stability is largely unaffected in the case of FFA and

GWO. The average value of the fitness function is the measure of the optimisation process efficiency, where a lower fitness function value corresponds to a better fit. In this regard, both FFA and GWO have average fitness function values in the range of  $10^{-4}$ , indicating their superior performance when compared to the MFO's average fitness function value, which is in the range of  $10^{13}$ .

The execution time of these algorithms too is also of interest since they have a direct bearing on the efficiency of the optimisation process. Therefore, when considering the execution time, MFO had the lowest average execution time of 8.32 seconds with a standard deviation of 0.6. GWO and MFO came second and third best in this regard with 38.86 and 241.29 seconds respectively. The standard deviations of the execution time too followed a similar trend. The results indicate that MFO sacrificed its accuracy and reliability for speed, while GWO emerges as the best option offering a combination of better fit, lower execution time and variation. Therefore, the initial parameter values have the lowest effect on the optimisation efficiency in the case of GWO, demonstrating its robustness towards initial values.

In the case of Pre-exponential factor, A, MFO has the highest average value ( $4.74 \times 10^{11}$ ) along with a large standard deviation ( $3.47 \times 10^{11}$ ), indicating much variability. FFA too produces similar results with the average value A and its standard deviation at  $4.32 \times 10^{11}$  and  $3.42 \times 10^{11}$  respectively. However, the average value of A as well as the standard deviation is the lowest in the case of GWO at  $2.18 \times 10^{11}$  and  $2.72 \times 10^{11}$  respectively.

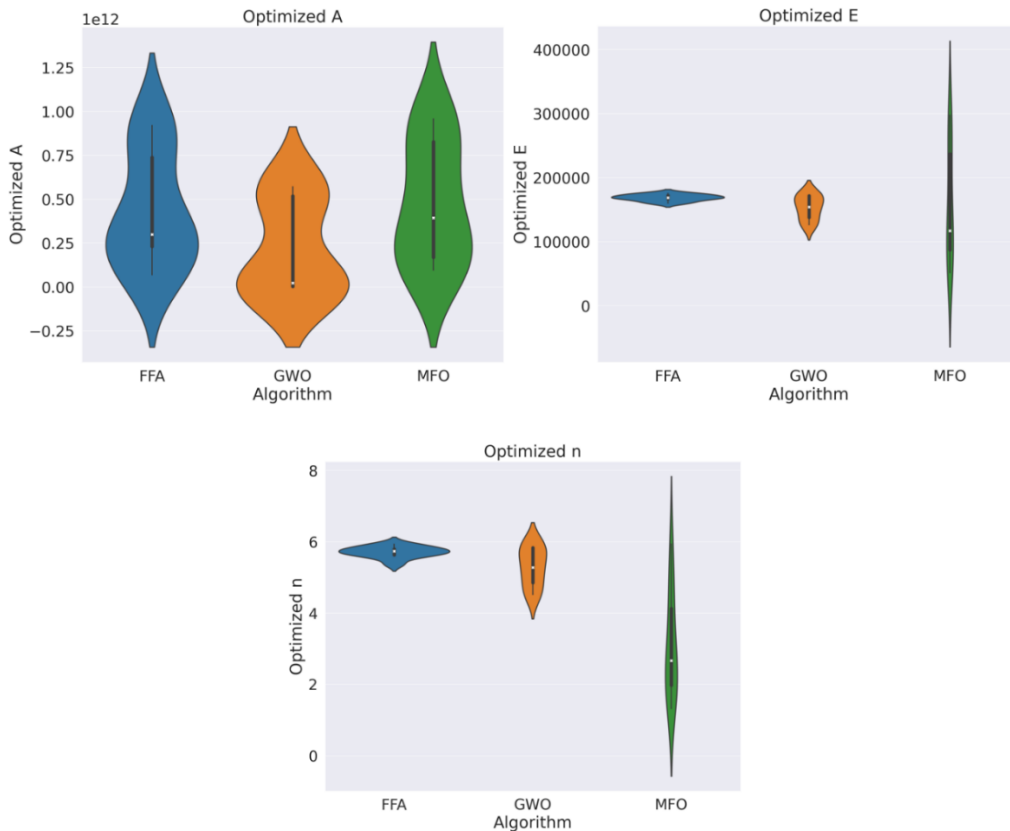
The results indicate that FFA predicts a higher energy barrier for the reaction on average, with the highest average value for the activation energy  $E_a$ ,  $16.8 \times 10^4$  J/mol. The standard deviation of  $5.04 \times 10^3$  indicates a low level of variability in  $E_a$ , indicating a consistent performance in activation energy estimation across several experiments. The Grey Wolf Optimizer (GWO) yields results with an average  $E_a$  of  $15.3 \times 10^4$  J/mol and a slightly higher standard deviation of  $18.7 \times 10^3$  J/mol. However, the MFO displays the highest standard deviation of  $91.8 \times 10^3$  indicating that its  $E_a$  estimations are most sensitive to the selection of initial parameters.

With a standard deviation of 1.5 for the reaction order n, MFO exhibits considerable variability, suggesting a notable variance in the values of n it determines. This might indicate that there is a wide range of possible reaction orders due to the significant sensitivity of MFO's model of the reaction mechanism to initial assumptions. However, the average n values for FFA and GWO cluster closer together, at 5.71 and 5.29, respectively, with FFA showing a narrower standard deviation of 0.159. This tightness implies that FFA consistently finds a comparable reaction sequence across several initializations, which might be advantageous for repeatability. Compared to FFA, but significantly less than MFO, GWO has a larger standard deviation to a certain extent for n (0.545), suggesting slightly more variability in the reaction order. These interpretations are corroborated by the violin plots shown in Figures 10 and 11.

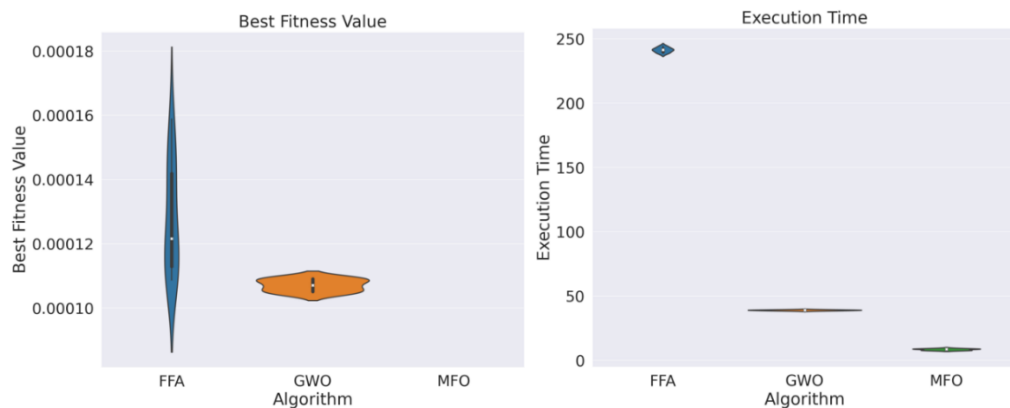
A Kernel Density Estimate (KDE) produces a smooth continuous curve where the width of the shape at different values represents the data's distribution density at that value. For instance, a wider part of a 'violin' means more data points exist at that value, while a narrower part means fewer data points.

The kernel density estimate (KDE) distributions visualize how optimized parameters like A,  $E_a$ , and n vary under the Firefly Algorithm (FFA) and Moth-Flame Optimization (MFO). The wider shape of the figures for the algorithms indicates the variations in the final values across the varied initial parameters. However, despite variations in starting inputs, the Grey Wolf Optimizer's (GWO) narrower KDE plots demonstrate more consistent optimisation of those parameters. This suggests that GWO is more resilient to changes in the initial values. Furthermore, for the optimal fitness value, the MFO shows the broadest KDE dispersion.

This wide dispersion points to erratic or inconsistent MFO optimisation performance. The narrowest violin shape is produced by the FFA in terms of execution time, indicating that it achieves more steady computation times than both GWO and MFO. GWO appears to be the most robust across multiple parameters, followed by FFA and MFO.



**Figure 10.** Violin plots visualizing the frequency of occurrence of the corresponding optimized values of parameters, A(Pre-Exponential Factor),  $E_a$ (Activation Energy), and n(order of reaction).



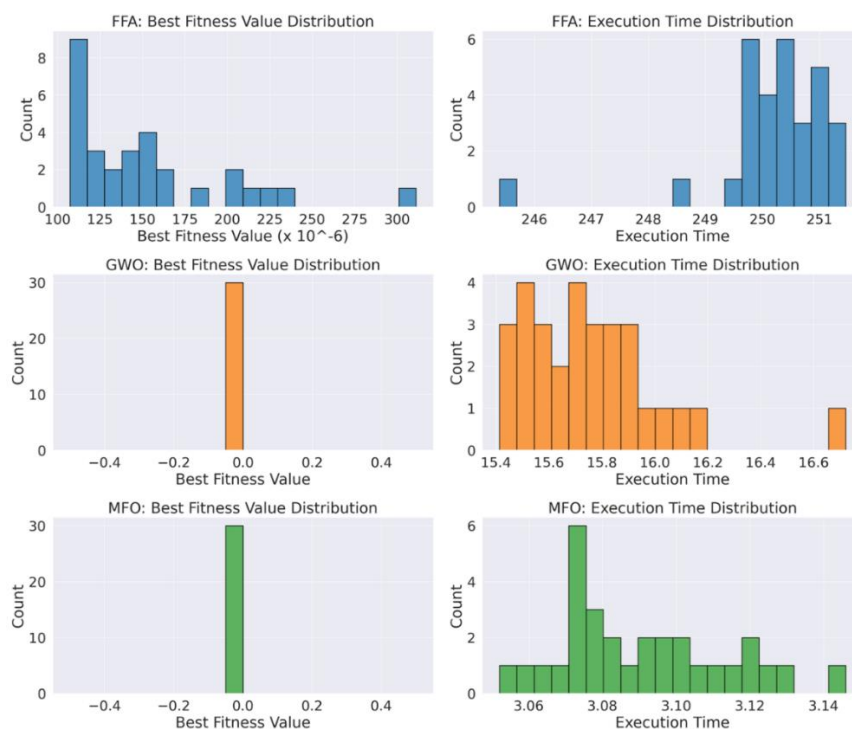
**Figure 11.** Violin plots visualizing the frequency of occurrence of the corresponding optimized values of fitness function values and execution time.

From all the above inferences, according to the robustness study, the most reliable method is the Grey Wolf Optimizer (GWO), which also has the most minor variability in fitness values and the lowest standard deviations for the estimated parameters  $A$ ,  $E_a$ , and  $n$ . This shows that it consistently finds the best answers under various initial circumstances. Moth-Flame Optimizer (MFO) exhibits substantial variability in fitness and the order of the reaction  $n$ , despite higher mean fitness values, raising concerns about its robustness. A balanced, albeit slower performance is delivered by the Firefly Algorithm (FFA) across all criteria. In particular, GWO stands out as the most reliable and effective option among the three algorithms since it not only delivers the most consistent and high-quality answers but also does so in the least amount of time.

#### 4.5 Repeatability Analysis

This study's main goal was to evaluate the repeatability of three metaheuristic optimization algorithms. Each algorithm used the same TGA dataset and attempted to estimate the kinetic parameters that best fit the data by minimizing an objective function that measured the sum of squared discrepancies between the experimental and modelled rate of conversion. To ensure a consistent and equitable evaluation, all algorithms were operated under identical conditions, each executed 30 times. The limits for the search agents were the same for all algorithms, with the lower limits set at  $[1e^3, 5e^4, 1]$  and upper limits at  $[1e^{12}, 3e^5, 6]$ . Every time a run was completed, the ideal kinetic parameters and their fitness values were recorded, collated into a Pandas DataFrame, and then saved as a CSV file. The study is well-positioned to directly compare the repeatability and performance of GWO, FFA, and MFO in optimizing TGA data by keeping this uniform approach in data processing, algorithm execution, and results recording.

The histograms in Figure 12 depict the distributions of best fitness values and execution times for each algorithm, providing intuitive insights into their performance metrics. Key statistics from the repeatability tests are listed in Table 5.



**Figure 12.** Distribution of the best fitness value and execution time for each algorithm.



**Table 5.** Key statistics from the repeatability tests.

Algorithm	Metric	Mean	Std Dev	Minimum	Maximum
Firefly Algorithm (FFA)	Best Fitness Value	$1.54 \times 10^{-4}$	$5.39 \times 10^{-5}$	$1.08 \times 10^{-4}$	$2.74 \times 10^{-4}$
	Execution Time (s)	244.33	4.84	236.41	257.32
Grey Wolf Optimizer (GWO)	Best Fitness Value	$1.05 \times 10^{-4}$	$6.36 \times 10^{-9}$	$1.05 \times 10^{-4}$	$1.05 \times 10^{-4}$
	Execution Time (s)	15.73	0.31	15.41	16.72
Moth Flame Optimizer (MFO)	Best Fitness Value	$1.28 \times 10^{-4}$	$2.16 \times 10^{-5}$	$1.05 \times 10^{-4}$	$1.86 \times 10^{-4}$
	Execution Time (s)	15.50	0.27	14.92	16.11

The histograms for best fitness values produced by the FFA are distributed across different ranges of values indicating that the algorithm might have a stochastic element inherent in its structure. Although the range of fitness values do suggest that the FFA can find optimal solutions albeit inconsistently. In contrast, GWO and MFO display very narrow spread. This implies that these algorithms are stable and consistent. When it comes to execution times, the FFA histogram reveals a broad range of execution times, indicating that there might be substantial variations in the amount of time needed for FFA to converge to a solution. While using FFA in time-sensitive applications, this fluctuation may be something to take into account. The distribution of execution times for GWO is more concentrated, suggesting more reliable computing performance. The time values are clustered in a narrow range, suggesting that GWO not only provides consistent optimization quality (as seen in the Best Fitness Value histogram) but also does so with predictable computational effort. MFO's execution times exhibit a distribution akin to its optimisation quality performance, but with a narrower spread than that of FFA. This suggests that MFO's problem-solving time varies to a moderate extent.

From Table 4, it is clear that GWO is the most repeatable of the three algorithms since it exhibits the least deviation in both optimal fitness values and execution times. This consistency could signify a more exploitative strategy, as it tends to provide similar results throughout different runs. On the other hand, the variation in FFA's results points to a predisposition for exploring various areas of the problem space. This can be helpful for thorough research, but it might not be the best option for situations requiring repeatability. The middle-ground results from MFO suggest a balanced strategy that combines exploration and exploitation.

Conclusively, the choice between FFA, GWO, and MFO hinges on the application's specific requirements. GWO emerges as the front-runner for situations where repeatability takes precedence over experimentation. On the other hand, tasks that emphasize thorough investigation might benefit from FFA's wide range. MFO, which sits in the middle of the two, looks ideal in situations looking for a delicate balance between exploration and exploitation.

#### 4.6 Parameter Tuning Analysis

This study engaged in a systematic comparison of three optimization algorithms in kinetic parameter estimation. The primary focus was understanding how varying hyperparameters affect the algorithms' performance, computational time, and result stability.

**Table 6.** Parameter tuning analysis input parameters.

Algorithm	Population Size	Iteration Range	Additional Parameters
Firefly Algorithm	[30, 50, 70]	[500, 1000, 1500, 2000]	Alpha: [0.1, 0.5, 1], Beta: [0.2, 1, 2], Gamma: [0.05, 0.5, 1]
Grey Wolf Optimizer	[30, 50, 70]	[500, 1000, 1500, 2000]	N/A
Moth Flame Optimizer	[30, 50, 70]	[500, 1000, 1500, 2000]	N/A

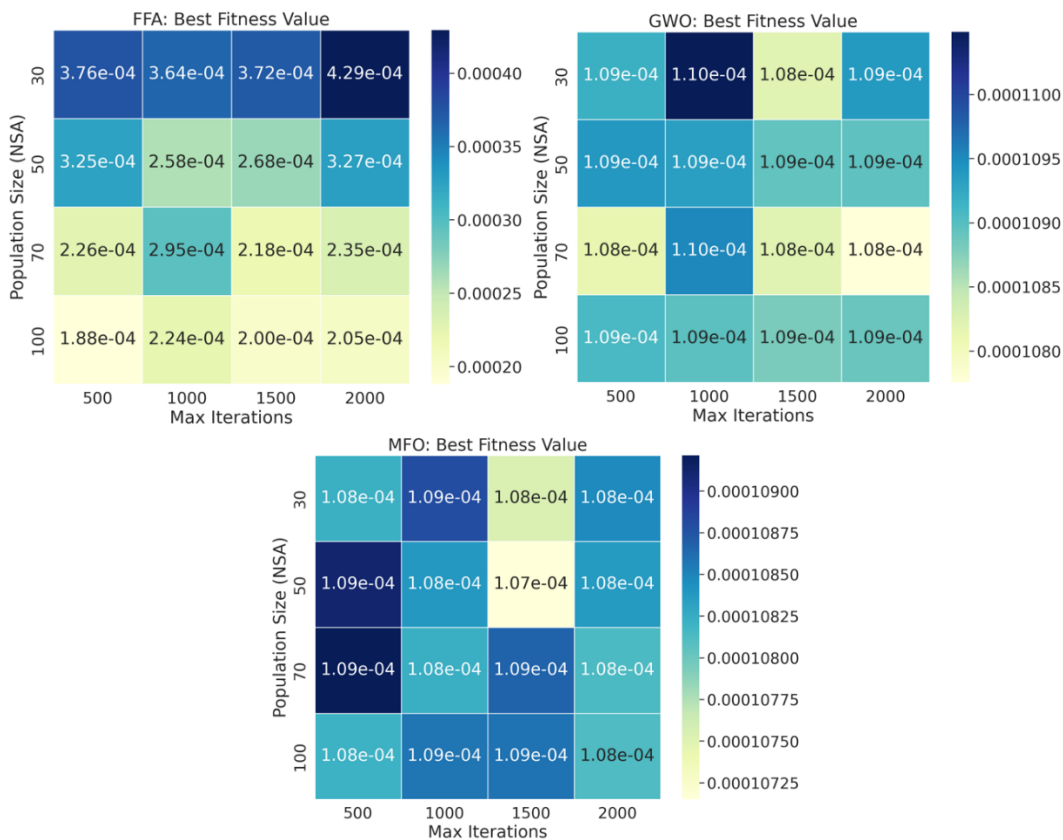
The algorithms were rigorously tested across multiple combinations of hyperparameters. Metrics like optimal kinetic parameters (A, E<sub>a</sub>, n), best fitness value, the number of iterations to converge, and computational time were tracked. Table 6 provides the design parameters of the parameter tuning analysis.

Results of the test runs are tabulated in Table 7 given below.

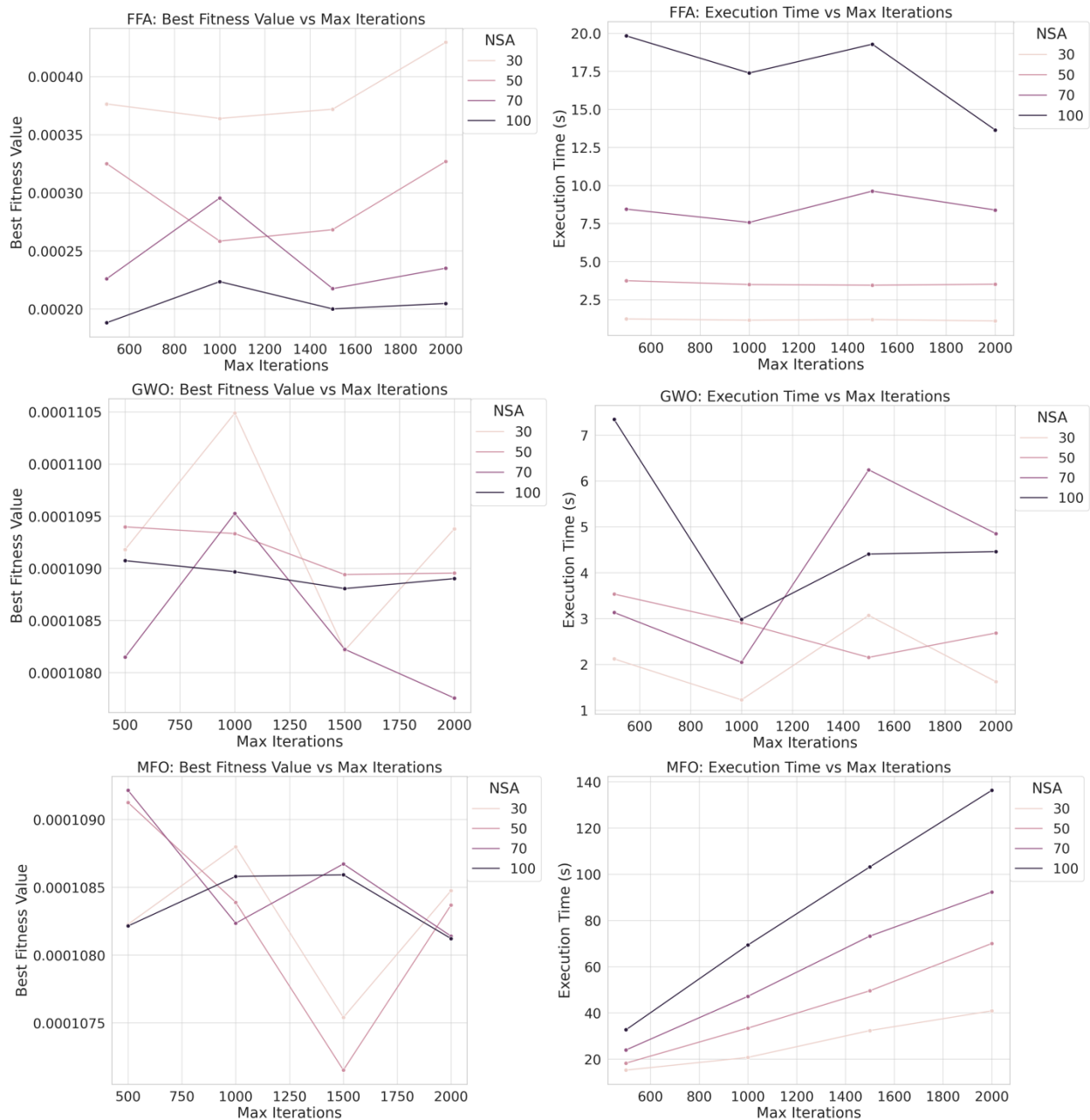
**Table 7.** Results of parameter tuning analysis.

Algorithm	Average Best Fitness Value	Std Dev of Best Fitness Value	Average Time Taken (seconds)	Std Dev of Time Taken (seconds)
FFA	$2.82 \times 10^{-4}$	$1.33 \times 10^{-4}$	7.69	7.59
GWO	$1.09 \times 10^{-4}$	$6.56 \times 10^{-7}$	3.42	1.67
MFO	$1.08 \times 10^{-4}$	$5.17 \times 10^{-7}$	53.65	34.53

A higher average fitness value of ( $2.82 \times 10^{-4}$ ) for the Firefly Algorithm (FFA) suggests that it might not be the best method for locating the global minimum in this optimization issue. Additionally, the higher standard deviation suggests less consistent results. The Grey Wolf Optimizer (GWO), on the other hand, showed a lower average fitness value ( $1.09 \times 10^{-4}$ ), indicating superior performance and a smaller standard deviation, resulting in a more stable set of results. The Moth Flame Optimizer (MFO) roughly matched GWO's performance with an average fitness value of ( $1.08 \times 10^{-4}$ ); however, its computational time was significantly higher, making it less efficient in terms of time complexity.



**Figure 13.** Heatmap of results highlighting the combination of parameter values providing the best fitness values in the parameter tuning analysis.



**Figure 14.** Line graph visualizing the relationship between fitness values and iterations categorized by the number of search agents.

The heatmaps and line graphs shown in Figures 13 and 14 provide a thorough overview of the performance metrics and computational time for each optimization procedure over a range of maximum iterations and population sizes (Number of Search Agents, NSA). Lighter colors indicate greater performance; the heatmaps expressly represent the average best fitness values. The line graphs simultaneously show the average best fitness values and the average time taken, segregated by NSA.

The heatmap and the line graph for the Firefly Algorithm (FA) confirm that larger population sizes and more iterations typically result in greater fitness scores. In contrast, as shown by its heatmap and line graph, the Grey Wolf Optimizer (GWO) maintains constant performance and demonstrates a lower average computational time throughout a range of population sizes and iterations.

In conclusion, Grey Wolf Optimizer (GWO) emerged as the most balanced algorithm in terms of performance and computational efficiency. It not only achieved the lowest average fitness values but did so in the least amount of time and with high result stability. Therefore, for the specific task of kinetic parameter estimation, GWO appears to be the most suitable algorithm among the three evaluated.

#### 4.7 Noise Analysis

The overarching objective of the study across all three optimization algorithms—Firefly Algorithm, Grey Wolf Optimizer, and Moth Flame Optimization—is to assess their robustness in handling uncertainties introduced as Gaussian noise. The algorithms aim to estimate kinetic parameters while minimizing the impact of the noise on the optimization process.

Three optimization algorithms were each given a function to introduce Gaussian noise to the input data to assess their coping ability. As the main criteria for optimization and robustness evaluation under noise, all algorithms used a single objective function that computes the sum of squares of the discrepancies between predicted and experimental conversion rates. FFA comprises of variables that include attractiveness, distance, and dynamic updates of locations which are examined for sensitivity towards noise. For GWO, position updates, and hierarchical components based on alpha, beta, and delta wolves were considered. The performance under noise of MFO which entails the dynamic updating of locations based on flame and moth positions, was evaluated.

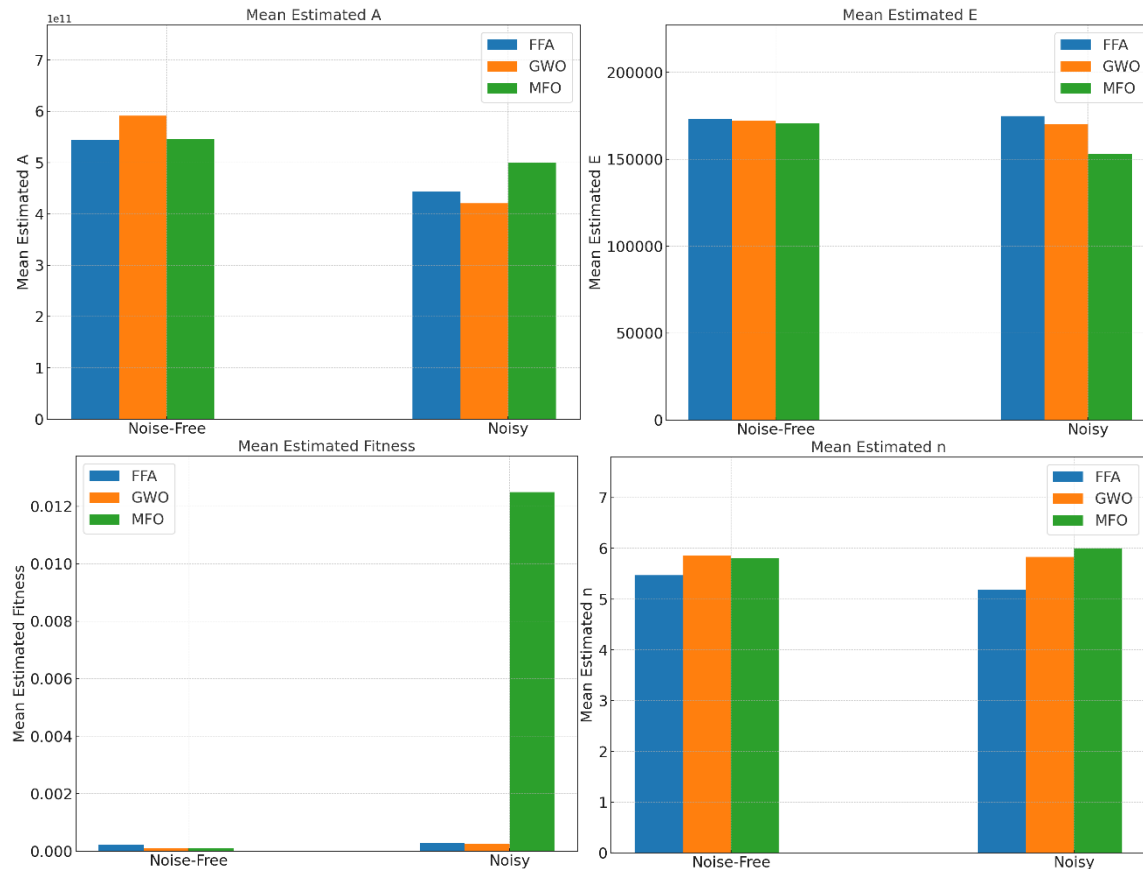
The main takeaways are a detailed comprehension of each method's robustness as demonstrated by performance fluctuations under noise and identifying the most reliable algorithm for kinetic parameter estimation in the face of imperfect data. The results from the test runs are provided in Table 8 given below.

**Table 8.** Results from noise handling analysis test run.

Algorithm	Data Type	Amean	Astd	Emean	Estd	nmean	nstd	Fitness Mean	Fitness Std
Firefly Optimizer (FFA)	noise-free	5.44×1011	3.24×1011	173118	5968	5.47	0.35	0.000227	1.0×10 <sup>-4</sup>
	noisy	4.44×1011	3.13×1011	174830	9241	5.19	0.59	0.000290	1.4×10 <sup>-4</sup>
Grey Wolf Optimizer (GWO)	noise-free	5.91×1011	0	172263	0	5.86	0	0.000109	0
	noisy	4.21×1011	0	170281	0	5.83	0	0.000255	0
Moth Flame Optimization (MFO)	noise-free	5.46×1011	3.50×1011	170589	4127	5.81	0.12	0.000109	6.76×10 <sup>-7</sup>
	noisy	5.00×1011	5.27×1011	153233	100573	6	0	0.0125	6.88×10 <sup>-5</sup>

From Table 7, it can be inferred that when noise is added to the data, the Grey Wolf Optimizer (GWO) and Firefly Algorithm (FFA) exhibit more robust tolerance to noise than Moth Flame Optimisation (MFO), as seen by their smaller increases in mean fitness values. In addition, GWO stands out for its stability, exhibiting 0% variation in fitness values, albeit this can mean the algorithm is locked in a local minimum. GWO leads the pack in terms of overall performance on noise-free data, having the lowest mean fitness, closely followed by MFO and, finally, FFA.

The performance of each method in both noise-free and noisy environments may be seen more thoroughly in visualizations using grouped bar graphs (Figure 15). Their robustness against noise may be carefully compared, contrasted, and understood with the help of this comprehensive presentation.



**Figure 15.** Visual representation of the variation in parameter values across data types (Noise-Free and Noisy).

From Figure 15 the overall trend can be seen in the bar graphs for the A, E, and n parameters: all algorithms operate best in a noise-free environment, although noise has varying effects on their capacity to optimise these parameters. Particularly FFA exhibits a discernible rise in the mean values of A and E when noise is present, suggesting a vulnerability to noise in data. Even though they are equally affected, GWO and MFO show less performance deterioration when noise is introduced, which may indicate stronger noise-handling capabilities. The most remarkable insights come from the bar plots when looking at fitness, the most important performance metric for these algorithms. Plots show that in both noisy and noise-free situations, GWO maintains the lowest mean fitness value, indicating a higher capacity to identify optimum solutions or more efficient convergence. The MFO exhibits a relative rise in fitness value in noisy situations, indicating that although it can still navigate toward optimum solutions, its accuracy and efficiency are lower than those of the GWO.

In conclusion, although the introduction of noise affects all three algorithms, GWO seems to be the most resilient, followed by FFA and MFO. In situations where the data may not be perfect, this makes GWO the most trustworthy method, even though its stability is a concern considering a zero standard deviation in

fitness values. Applying FFA and MFO to noisy data sets may require additional modifications or considerations.

## 5. Conclusion, Recommendations and Limitations

In this study, we carried out a thorough analysis of the Firefly Algorithm (FFA), Grey Wolf Optimizer (GWO), and Moth Flame Optimizer (MFO) focusing on their performance in estimating the kinetic parameters for a single-step coal pyrolysis model. The main objective was to evaluate the applicability of these methods for optimizing the model's parameters and to offer insight into their strengths and weaknesses.

Our findings reveal that all three algorithms effectively estimated kinetic parameters by fitting data, showcasing their accuracy. The FFA and MFO yielded really good results, with fitness values of  $1.09 \times 10^{-4}$  and  $1.04 \times 10^{-4}$ . However, the best performer was the GWO, which fared better to a certain extent with a fitness value of  $1.04 \times 10^{-4}$ . Meanwhile, the MFO algorithm was the fastest in terms of computation time (113.4 seconds), making it a good choice where processing speed is essential. Upon examining the specifics of every algorithm, the MFO estimated the highest values for activation energy  $E_a$ , pre-exponential factor  $A$  and reaction order  $n$ . However, each algorithm's convergence rate varied, FFA had the slowest convergence rate (-0.057), lowering fitness values starting from 0.000474 at the beginning to 0.000447 at the end. The Grey Wolf Optimizer (GWO) showed a far more aggressive convergence, as evidenced by a -0.625 convergence rate and a fitness value that fell from 0.000280 to 0.000105. This suggests a rapid and significant improvement in its optimisation performance. Finally, a modest optimisation progress was shown by the Moth Flame Optimizer (MFO), which showed a minor improvement from 0.000128 to 0.000108 with a convergence rate of -0.156. In summary convergence rate analysis quantified the GWO's rapid improvements to the fitness values indicating its suitability to problems requiring quick solutions.

In our robustness test analysis, we found that even with varied initial parameters, all three algorithms consistently converge to similar solutions. The average kinetic and fitness values across several runs highlight the effectiveness of the algorithms. However, standard deviations in fitness values revealed differing stability and accuracy retention. The standard deviations for fitness values show a reasonable variance for FFA ( $10^{-5}$ ) and GWO ( $10^{-6}$ ), but a substantial variability for MFO ( $10^{14}$ ). When it comes to average fitness function values, MFO's average is much less ideal at  $10^{13}$ , although FFA and GWO both report in the  $10^{-4}$  range, demonstrating their efficiency. When it comes to execution times, GWO and FFA come in second and third, with 38.86 and 241.29 seconds respectively, with MFO leading with the smallest average of 8.32 seconds ( $\pm 0.6$  SD). This implies that during the optimisation process, FFA and GWO retain greater accuracy and stability while MFO sacrifices accuracy and robustness for speed.

GWO also demonstrated the greatest repeatability, providing consistent outcomes across several runs, with the lowest standard deviation across the three algorithms at  $6.36 \times 10^{-9}$ . Even the average value of the fitness function was the lowest for GWO at  $1.05 \times 10^{-4}$ . While MFO established a balance between exploration and exploitation, FFA displayed unpredictability, suggesting a propensity to investigate different solution spaces. To sum up, FFA is more appropriate for situations requiring extensive investigation, but GWO is the recommended approach where consistency and repeatability are critical. MFO is a good choice for activities that require a careful balance between the two techniques since it offers an ideal combination of exploration and exploitation.

In terms of parameter tuning analysis, GWO balanced speed (3.42 seconds) and efficiency (avg. fitness values of  $1.09 \times 10^{-4}$  and  $\pm 6.56 \times 10^{-7}$  SD), whereas MFO computed more slowly even if its performance was comparable (avg. fitness values of  $1.08 \times 10^{-4}$ ). These algorithms also displayed strong resilience to noise in

data. The Firefly Algorithm (FFA) demonstrated steady performance even in the presence of noise, with the fitness standard deviation rising just slightly from  $1.0 \times 10^{-4}$  to  $1.4 \times 10^{-4}$ . Remarkably the Grey Wolf Optimizer (GWO) demonstrated perfect noise tolerance, as seen by zero fitness values for both noisy and noise-free data. The Moth Flame Optimisation (MFO), on the other hand, showed significant sensitivity when switching from noise-free to noisy data. Its mean fitness dropped from 0.000109 to 0.0125, and the standard deviation rose to  $6.88 \times 10^{-5}$ . To sum up, data noise had a major effect on the MFO, a little impact on the FFA, and a minimal impact on the stable optimisation of the GWO. This indicates that the MFO has the highest sensitivity and the GWO is the most noise robust technique.

Based on our comprehensive analysis, we recommend the Moth Flame Optimizer (MFO) for rapid convergence needs in time-sensitive applications, the Firefly Optimizer (FFA) for applications requiring extensive explorations and the Grey Wolf Optimizer (GWO) for its reliability and consistency overall. Apart from the speed of execution, GWO was the best performer in terms of robustness to initial parameter values, consistent repeatability, and resilience to noise in the data.

This study contributes to understanding metaheuristic optimization algorithms' applicability in estimating kinetic parameters for coal pyrolysis models. We improve the subject of coal pyrolysis modeling and optimization by providing essential information to researchers and practitioners so they may choose an algorithm for their particular needs with knowledge of its performance characteristics. The choice of algorithm ultimately depends on the specific demands of the task, as each algorithm has demonstrated its unique strengths and characteristics.

While this study has merit, there are some restrictions that could be addressed by further research on the topic. The present investigation highlights the dependence of the efficacy of the FFA, GWO, and MFO algorithms on the particular configurations and starting parameter estimations, which may not translate to other models or problem definitions. The performance metrics, influenced by the search space size and the landscape of the objective function, may not reflect all potential operational scenarios, posing a limitation to their broader application. Moreover, the evaluations of robustness and repeatability were carried out under limited conditions, which might not fully accommodate the range of real-world fluctuations. Additionally, the algorithms' sensitivity to hyperparameter adjustment raises the possibility of an impact on transferability and usability. Due to its overall high performance, the GWO is advised for general usage; however, this recommendation is accompanied by a caveat that it might not be ideal for every single purpose. This highlights how crucial it is to properly verify that the algorithms are appropriate for the particular scenario at hand.

Although our study offers insightful information, there is room for more investigation and prospective advancements. Hybridization of algorithms is one of the main aspects. The advantages of combining various metaheuristic algorithms to maximize their strengths and minimize their flaws must be investigated. Real-world applications of these metaheuristic algorithms in coal pyrolysis or other domains could provide valuable insights into their practical utility. Developing noise-handling techniques or adjustments will make FFA and MFO more robust to noisy data. It is recommended to investigate the parallelization strategies to speed up the optimization process even further.

#### **Conflict of Interest**

The authors confirm that there is no conflict of interest to declare for this publication.

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### References

- Abdelouahed, L., Leveneur, S., Vernieres-Hassimi, L., Baland, L., & Taouk, B. (2017). Comparative investigation for the determination of kinetic parameters for biomass pyrolysis by thermogravimetric analysis. *Journal of Thermal Analysis and Calorimetry*, 129(2), 1201-1213. <https://doi.org/10.1007/s10973-017-6212-9>.
- Aghbashlo, M., Tabatabaei, M., Nadian, M.H., Davoodnia, V., & Soltanian, S. (2019). Prognostication of lignocellulosic biomass pyrolysis behavior using ANFIS model tuned by PSO algorithm. *Fuel*, 253, 189-198. <https://doi.org/10.1016/j.fuel.2019.04.169>.
- Cai, J., Wu, W., & Liu, R. (2012). Isoconversional kinetic analysis of complex solid-state processes: Parallel and successive reactions. *Industrial & Engineering Chemistry Research*, 51(49), 16157-16161. <https://doi.org/10.1021/ie302160d>.
- Dhyani, V., & Bhaskar, T. (2018). Chapter 2-Kinetic analysis of biomass pyrolysis. In: Bhaskar, T., Pandey, A., Mohan, S.V., Lee, D.J., Khanal, S.K. (eds) *Waste Biorefinery*. Elsevier, pp. 39-83. <https://doi.org/10.1016/b978-0-444-63992-9.00002-1>.
- Ding, Y., Huang, B., Li, K., Du, W., Lu, K., & Zhang, Y. (2020). Thermal interaction analysis of isolated hemicellulose and cellulose by kinetic parameters during biomass pyrolysis. *Energy*, 195, 117010. <https://doi.org/10.1016/j.energy.2020.117010>.
- Ding, Y., Zhang, W., Yu, L., & Lu, K. (2019). The accuracy and efficiency of GA and PSO optimization schemes on estimating reaction kinetic parameters of biomass pyrolysis. *Energy*, 176, 582-588. <https://doi.org/10.1016/j.energy.2019.04.030>.
- Duan, Q.Y., Gupta, V.K., & Sorooshian, S. (1993). Shuffled complex evolution approach for effective and efficient global minimization. *Journal of Optimization Theory and Applications*, 76(3), 501-521. <https://doi.org/10.1007/bf00939380>.
- Ferreiro, A.I., Rabaçal, M., & Costa, M. (2016). A combined genetic algorithm and least squares fitting procedure for the estimation of the kinetic parameters of the pyrolysis of agricultural residues. *Energy Conversion and Management*, 125, 290-300. <https://doi.org/10.1016/j.enconman.2016.04.104>.
- Jain, A.A., Mehra, A., & Ranade, V.V. (2016). Processing of TGA data: Analysis of isoconversional and model fitting methods. *Fuel*, 165, 490-498. <https://doi.org/10.1016/j.fuel.2015.10.042>.
- Khan, M., Ullah, Z., Mašek, O., Raza Naqvi, S., & Nouman Aslam Khan, M. (2022). Artificial neural networks for the prediction of biochar yield: A comparative study of metaheuristic algorithms. *Bioresour Technol*, 355, 127215. <https://doi.org/10.1016/j.biortech.2022.127215>.
- Khare, P., Baruah, B.P., & Rao, P.G. (2011). Application of chemometrics to study the kinetics of coal pyrolysis: A novel approach. *Fuel*, 90(11), 3299-3305. <https://doi.org/10.1016/j.fuel.2011.05.017>.
- Kök, M.V. (2002). Thermal analysis applications in fossil fuel science: Literature survey. *Journal of Thermal Analysis and Calorimetry*, 68(3), 1061-1077. <https://doi.org/10.1023/a:1016119428815>.
- Kok, M.V., & Okandan, E. (1995). Kinetic analysis of in situ combustion processes with thermogravimetric and differential thermogravimetric analysis and reaction tube experiments. *Journal of Analytical and Applied Pyrolysis*, 31, 63-73. [https://doi.org/10.1016/0165-2370\(94\)00812-f](https://doi.org/10.1016/0165-2370(94)00812-f).
- Kumar, A., Pant, S., & Ram, M. (2017). System Reliability optimization using gray wolf optimizer algorithm. *Quality and Reliability Engineering International*, 33(7), 1327-1335. <https://doi.org/10.1002/qre.2107>.



- Kumar, A., Pant, S., Ram, M., & Chaube, S. (2019). Multi-objective grey wolf optimizer approach to the reliability-cost optimization of life support system in space capsule. *International Journal of System Assurance Engineering and Management*, 10(2), 276-284. <https://doi.org/10.1007/s13198-019-00781-1>.
- Kumar, A., Pant, S., Ram, M., & Yadav, O. (2022). *Meta-heuristic optimization techniques: Applications in engineering*. Walter de Gruyter GmbH & Co KG, Berlin / Boston.
- Lautenberger, C., & Fernandez-Pello, A.C. (2011). Optimization algorithms for material pyrolysis property estimation. *Fire Safety Science*, 10, 751-764. <https://doi.org/10.3801/iafss.fss.10-751>.
- Li, C., Dai, Z.H., Yang, J., Yu, G.S., & Wang, F.C. (2015). Modelling and energy analysis of an integrated coal gasification and pyrolysis system for synthetic natural gas. *Journal of Fuel Chemistry and Technology*, 43(7), 779-789. [https://doi.org/10.1016/s1872-5813\(15\)30024-4](https://doi.org/10.1016/s1872-5813(15)30024-4).
- Lu, K.M., Lee, W.J., Chen, W.H., & Lin, T.C. (2013). Thermogravimetric analysis and kinetics of co-pyrolysis of raw/torrefied wood and coal blends. *Applied Energy*, 105, 5-65. <https://doi.org/10.1016/j.apenergy.2012.12.050>.
- Meng, Z., Li, G., Wang, X., Sait, S.M., & Yıldız, A.R. (2021). A comparative study of metaheuristic algorithms for reliability-based design optimization problems. *Archives of Computational Methods in Engineering*, 28(3), 1853-1869. <https://doi.org/10.1007/s11831-020-09443-z>.
- Mirjalili, S. (2015). Moth-flame optimization algorithm: A novel nature-inspired heuristic paradigm. *Knowledge-Based Systems*, 89, 228-249. <https://doi.org/10.1016/j.knsys.2015.07.006>.
- Mirjalili, S., Mirjalili, S.M., & Lewis, A. (2014). Grey wolf optimizer. *Advances in Engineering Software*, 69, 46-61. <https://doi.org/10.1016/j.advengsoft.2013.12.007>.
- Negi, G., Kumar, A., Pant, S., & Ram, M. (2021). Optimization of complex system reliability using hybrid grey wolf optimizer. *Decision Making: Applications in Management and Engineering*, 4(2), 241-256. <https://doi.org/10.31181/dmame210402241n>.
- Pant, S., Kumar, A., & Ram, M. (2019). Solution of nonlinear systems of equations via metaheuristics. *International Journal of Mathematical, Engineering and Management Sciences*, 4(5), 1108-1126. <https://doi.org/10.33889/10.33889/ijmems.2019.4.5-088>.
- Sakthivel, R., Harshini, G.V., Vardhan, M.S., Vinod, A., & Gomathi, K. (2023). 3-Biomass energy conversion through pyrolysis: A ray of hope for the current energy crisis. In: Singh, V.K., Bangari, N., Tiwari, R., Dubey, V., Bhoi, A.K., & Babu, T.S. (eds) *Green Energy Systems*. Academic Press, pp. 37-68. <https://doi.org/10.1016/b978-0-323-95108-1.00006-9>.
- Sauerbrunn, S., & Gill, P. (1994). Decomposition kinetics using TGA. *American Laboratory*, 26, 29-29.
- Schobert, H.H., & Song, C. (2002). Chemicals and materials from coal in the 21st century. *Fuel*, 81(1), 15-32. [https://doi.org/10.1016/s0016-2361\(00\)00203-9](https://doi.org/10.1016/s0016-2361(00)00203-9).
- Skreiberg, A., Skreiberg, O., Sandquist, J., & Sørum, L. (2011). TGA and macro-TGA characterisation of biomass fuels and fuel mixtures. *Fuel*, 90(6), 2182-2197. <https://doi.org/10.1016/j.fuel.2011.02.012>.
- Solomon, P.R., Serio, M.A., & Suuberg, E.M. (1992). Coal pyrolysis: Experiments, kinetic rates and mechanisms. *Progress in Energy and Combustion Science*, 18(2), 133-220. [https://doi.org/10.1016/0360-1285\(92\)90021-r](https://doi.org/10.1016/0360-1285(92)90021-r).
- Song, H., Liu, G., & Wu, J. (2016). Pyrolysis characteristics and kinetics of low rank coals by distributed activation energy model. *Energy Conversion and Management*, 126, 1037-1046. <https://doi.org/10.1016/j.enconman.2016.08.082>.
- Song, H., Liu, G., Zhang, J., & Wu, J. (2017). Pyrolysis characteristics and kinetics of low rank coals by TG-FTIR method. *Fuel Processing Technology*, 156, 454-460. <https://doi.org/10.1016/j.fuproc.2016.10.008>.

- Stauffer, E., Dolan, J.A., & Newman, R. (2008). Chapter 4-Chemistry and physics of fire and liquid fuels. In: Stauffer, E., Dolan, J.A., & Newman, R. (eds) *Fire Debris Analysis*. Academic Press, pp. 85-129. <https://doi.org/10.1016/b978-012663971-1.50008-7>.
- Till, Z., Chován, T., & Varga, T. (2020). Improved understanding of reaction kinetic identification problems using different nonlinear optimization algorithms. *Journal of the Taiwan Institute of Chemical Engineers*, 111, 73-79. <https://doi.org/10.1016/j.jtice.2020.05.013>.
- Ullah, Z., Khan, M., Naqvi, S.R., Khan, M.N.A., Farooq, W., Anjum, M.W., Yaqub, M.W., AlMohamadi, H., & Almomani, F. (2022). An integrated framework of data-driven, metaheuristic, and mechanistic modeling approach for biomass pyrolysis. *Process Safety and Environmental Protection*, 162, 337-345. <https://doi.org/10.1016/j.psep.2022.04.013>.
- Uniyal, N., Pant, S., & Kumar, A. (2020). An overview of few nature inspired optimization techniques and its reliability applications. *International Journal of Mathematical, Engineering and Management Sciences*, 5(4), 732-743. <https://doi.org/10.33889/ijmems.2020.5.4.058>.
- van Heek, K.H., & Hodek, W. (1994). Structure and pyrolysis behaviour of different coals and relevant model substances. *Fuel*, 73(6), 886-896. [https://doi.org/10.1016/0016-2361\(94\)90283-6](https://doi.org/10.1016/0016-2361(94)90283-6).
- Vyazovkin, S. (2018). Chapter 4 - Modern isoconversional kinetics: from misconceptions to advances. In: Vyazovkin, S., Koga, N., & Schick, C. (eds) *Handbook of Thermal Analysis and Calorimetry* (vol. 6, pp. 131-172). Elsevier <https://doi.org/10.1016/b978-0-444-64062-8.00008-5>.
- Wang, C., Zhang, X., Liu, Y., & Che, D. (2012). Pyrolysis and combustion characteristics of coals in oxyfuel combustion. *Applied Energy*, 97, 264-273. <https://doi.org/10.1016/j.apenergy.2012.02.011>.
- Webster, R.D. (2009). *Pyrolysis model parameter optimization using a customized stochastic hill-climber algorithm and bench scale fire test data* [M.S., University of Maryland, College Park].
- Xu, L., Jiang, Y., & Wang, L. (2017). Thermal decomposition of rape straw: Pyrolysis modeling and kinetic study via particle swarm optimization. *Energy Conversion and Management*, 146, 124-133. <https://doi.org/10.1016/j.enconman.2017.05.020>.
- Yan, J., Liu, M., Feng, Z., Bai, Z., Shui, H., Li, Z., Lei, Z., Wang, Z., Ren, S., Kang, S., & Yan, H. (2020). Study on the pyrolysis kinetics of low-medium rank coals with distributed activation energy model. *Fuel*, 261, 116359. <https://doi.org/10.1016/j.fuel.2019.116359>.
- Yang, H., Yan, R., Chen, H., Lee, D.H., & Zheng, C. (2007). Characteristics of hemicellulose, cellulose and lignin pyrolysis. *Fuel*, 86(12-13), 1781-1788. <https://doi.org/10.1016/j.fuel.2006.12.013>.
- Yang, X.S. (2009). Firefly algorithms for multimodal optimization. In: O. Watanabe & T. Zeugmann (eds) *Stochastic algorithms: Foundations and Applications*. SAGA 2009. Lecture Notes in Computer Science (Vol. 5792, pp. 169-178). Springer, Berlin, Heidelberg. [https://doi.org/10.1007/978-3-642-04944-6\\_14](https://doi.org/10.1007/978-3-642-04944-6_14).
- Yu, J., Shi, L., Liu, Z., Qin, X., Liu, M., & Liu, Q. (2023). Behaviors of coking and kinetics of volatiles' reaction during coal pyrolysis in a two-stage reactor. *Journal of Analytical and Applied Pyrolysis*, 173, 106050. <https://doi.org/10.1016/j.jaap.2023.106050>.
- Zhang, L., Xu, C.C., & Champagne, P. (2010). Overview of recent advances in thermo-chemical conversion of biomass. *Energy Conversion and Management*, 51(5), 969-982. <https://doi.org/10.1016/j.enconman.2009.11.038>.

