Hybrid Complex Proportional Assessment-Multi-objective Grey Wolf Optimizer for Biodiesel Process Optimization

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Abstract. In this study, a hybrid COPRAS-MOGWO (Complex Proportional Assessment-Multi-Objective Grey Wolf Optimizer) optimization approach is proposed for optimizing biodiesel production. The performance of the MOGWO is compared with Non-dominated Sorting Genetic Algorithm II (NSGA-II). Optimization of biodiesel production from waste frying soybean oil through transesterification is considered as the case study to test the proposed algorithm. The research aims to minimize energy consumption and maximize reaction conversion and green chemistry balance simultaneously. Results indicate that MOGWO outperforms NSGA-II in terms of computational time and solution quality. Furthermore, the same best compromise solution (BCS) is identified by COPRAS across different weight-based scenarios. By comparing the relative performance of NSGA-II and MOGWO, this study contributes valuable insights into multi-objective optimization in biodiesel production and provides guidance for researchers and practitioners in selecting appropriate optimization algorithms to improve the efficiency and sustainability of biodiesel production processes.

Keywords: Optimization · multi-objective · multi-criteria · compromise solution

1 Introduction

Biodiesel is a type of fuel that is produced from the esters of long-chain fatty acids found in animals and plants. Biodiesel is a rapidly growing alternative fuel that shares many properties with fossil diesel. It is easy to produce, biodegradable, non-toxic, and poses no threat to human health. These characteristics make it a popular choice for those seeking a sustainable fuel option. The harmful pollutants emitted from burning diesel

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have led researchers to explore alternative sources with similar characteristics while reducing diesel consumption through blending with alternative fuels. A key advantage of biodiesel is its ability to integrate smoothly into the current vehicle infrastructure, necessitating only minimal modifications to the system. Biodiesel also contributes to sustainability in various industries involved in power generation, transportation, and heat generation. Biodiesel offers diversity across the three pillars of sustainable development: energy, economy, and environment. This renewable fuel can be produced domestically using various resources, including cooking oil [1], soybean oil [2], animal fat, and plant waste, providing alternative sources to edible oil in biodiesel production [3]. Biodiesel is also safe to handle and transport, and it has been approved by the Environmental Protection Agency (EPA) as an alternative fuel. Additionally, it does not contain sulfur, which can prolong the life of emission-reducing devices and catalytic converters. The transesterification process, which involves reacting parent oil with alcohol in the presence of catalysts like KOH [4] or NaOH [5], is used to produce biodiesel. To maximize the biodiesel yield from different bio-oils, several parameters must be optimized, including the amount of catalyst, reaction time, reaction temperature, and methanol-to-oil molar ratio.

Rajendiran et al. [6] worked on producing biodiesel using Calophyllum inophyllum oil and zinc-doped calcium oxide mixed with methanol. The Calophyllum inophyllum oil contains free fatty acids, which were treated with 0.5% sulfuric acid and a methanol-to-oil molar ratio of 4:1 at 60 °C for 120 min. After undergoing magnetic stirring, heating, and separation processes, glycerine was separated from the crude biodiesel. Chattopadhyay et al. [7] studied biocatalytic biodiesel production from cottonseed oil using low-cost crude pancreatic lipase as a catalyst. They achieved maximum biodiesel conversion at a reaction time of 4 h, a methanol-to-oil molar ratio of 1:15, and a reaction temperature of 37 °C.

Various optimization methods, such as face-centered central composite design (FCCD), Box-Behnken design (BBD), central composite design (CCD), and response surface methodology (RSM), are used to obtain experimental design results. Ahmad et al. [8] used RSM to achieve the maximum biodiesel yield through the transesterification reaction of flaxseed oil, predicting a 99.5% biodiesel yield at a reaction temperature of 59 °C, reaction time of 33 min, and 0.51% catalyst concentration. Balaji et al. [9] employed a central composite design-based response surface methodology to maximize the predicted value of 99.23% biodiesel yield under optimal conditions, such as 2.68 weight percentage of calcined red banana peduncle (CRBP) concentration, 11.46:1 methanol-to-esterified Ceiba pentandra oil (E-CPO) molar ratio, and a reaction time of 106 min. Jamshaid et al. [10] used the central composite rotatable design of experiment methodology with RSM to optimize production process parameters. They found the optimum conditions for a maximum yield of 98.3% Cottonseed Oil Methyl Ester to be a catalyst weight percentage of 0.97%, a methanol-to-oil molar ratio of 6:1, and a reaction temperature of 63 °C. Cabello et al. worked on optimizing solid waste food oil using ultrasound-assisted transesterification. They employed the RSM optimization method to perform the design of experiments. Optimal conditions for the esterification reaction were a methanol-to-oil molar ratio of 6.08:1, a weight percentage of 1.28, and a reaction temperature of 52.5 °C, resulting in a maximum yield percentage of 93.23.

Nayak et al. [11] demonstrated the optimization of microwave-assisted biodiesel production from papaya oil using response surface methodology. Papaya oil was investigated under 700W microwave power with constant magnetic stirring. The optimized operating conditions were a methanol-to-oil molar ratio of 9.50:1, a catalyst temperature of 62.33 °C, a reaction time of 3.30 min, and a catalyst weight percentage of 0.95. The predicted biodiesel yield was 99.9% through RSM optimization, while the experimentally determined yield was 99.3%.

In a study by Goncalves et al. [12], multi-objective optimization (MOO) was employed to enhance biodiesel flow rate and reduce energy consumption in the production process. The team utilized process simulation and discovered that the optimal conditions for achieving these objectives depend on the weight assigned to each individual objective function. They also found that reactor temperature had a more significant impact on biodiesel production than energy consumption. De et al. [13] also explored multi-objective optimization in integrated biodiesel production and separation systems. They formulated two MOO problems (MOOP1 and MOOP2) to examine the trade-offs among performance indices of the reactor and separation units. MOOP2 produced more cost-effective results in terms of comprehensive trade-offs among the objective functions used, determining that the energy expenditure in the reactor jacket was 1.064 times the total energy usage of all reboilers in the distillation column.

While significant progress has been made in the field of biodiesel production optimization, a research gap remains in the area of multi-objective optimization algorithm comparisons for simultaneous minimization of energy consumption and maximization of reaction conversion and green chemistry balance. Current literature has mostly focused on optimization techniques for individual aspects of biodiesel production, such as yield, catalyst selection, and reaction parameters. However, a comprehensive analysis of multi-objective optimization algorithms and their performance in addressing these objectives simultaneously is still lacking.

The contribution of this research paper is to address this gap by comparing the performance of two well-known multi-objective optimization algorithms, NSGA-II and MOGWO, in optimizing the biodiesel production process. The research evaluates the algorithms' effectiveness in identifying non-dominated solutions (NDS) that minimize energy consumption and maximize reaction conversion and green chemistry balance. The study employs a case study from the literature by Outili et al. [14] to provide a context for the algorithm comparison. The research also utilizes the COPRAS method to quantitatively compare the NDS solutions of NSGA-II and MOGWO, highlighting the differences in their performance under various weight-based scenarios.

By evaluating the relative performance of NSGA-II and MOGWO, this paper adds valuable insights to the field of multi-objective optimization in biodiesel production. Furthermore, the results of this study may guide researchers and practitioners in selecting appropriate optimization algorithms for biodiesel production processes, ultimately leading to more efficient and sustainable production methods.

The paper is structured as follows: Sect. 1 provides an overview of the research topic, background information and the objectives of the study. Section 2 contains the details regarding the experimental setup, NSGA-II algorithm and MOGWO algorithm. Section 3 deals with the optimal prediction with NSGA-II and MOGWO as well as

their comparative analysis. Finally, Sect. 4 presents the Conclusion, summarizing the key findings of the research and their implications.

2 Materials and Methods

2.1 Experimental Details

In this study, a case study from the literature, based on the work of Outili et al. [14], is considered. Outili et al. [14] produced biodiesel from waste frying soybean oil collected from restaurants using the transesterification reaction. Their goal was to reduce energy and reactant consumption, as well as waste generation, in order to achieve a greener process. A multi-objective optimization employing the central composite design (CCD) was carried out, taking into account three responses: reaction conversion, energy consumption, and green chemistry balance. Temperature (X_1), KOH catalyst amount (X_2), and oil-to-methanol molar ratio (X_3) served as the independent variables in the CCD. Quadratic models for the responses (reaction conversion, energy consumption, and green chemistry balance) are detailed below

$$\begin{aligned}\text{Reaction Conversion} &= 0.999841 + 0.002115X_1 + 0.012355X_2 + 0.024807X_3 \\ &+0.001039X_1^2 - 0.001514X_2^2 - 0.019388X_3^2 - 0.003611X_1X_2 - 0.003611X_1X_3 \\ &-0.018056X_2X_3\end{aligned} \tag{1}$$

$$\text{Energy Consumption} = 3.826 + 0.555X_1 - 0.056X_2 + 0.148X_3 + 0.019X_1X_3 \tag{2}$$

$$\begin{aligned}\text{Green chemistry balance} &= 0.718780 - 0.004789X_1 - 0.009939X_2 \\ &-0.038683X_3 + 0.004788X_1^2 + 0.006372X_2^2 - 0.001711X_3^2 \\ &-0.005753X_1X_2 - 0.000243X_1X_3 + 0.001019X_2X_3\end{aligned} \tag{3}$$

The objective is to minimize the energy consumption while maximizing the reaction conversion and green chemistry balance.

2.2 NSGA-II

NSGA-II, or Non-dominated Sorting Genetic Algorithm II, is an evolutionary multi-objective optimization algorithm developed by Kalyanmoy Deb and his colleagues in 2002 [15]. This algorithm is an extension of the original Non-dominated Sorting Genetic Algorithm (NSGA) and aims to solve complex optimization problems involving multiple conflicting objectives. The various key features of NSGA-II are as follows.

- Fast Non-dominated Sorting: NSGA-II employs an efficient non-dominated sorting method, which is the process of classifying solutions into different levels of non-domination, called fronts. This method ensures that the best solution sets, which do not dominate one another, are promoted in the algorithm's search.
- Elitism: One of the main improvements of NSGA-II over its predecessor is the incorporation of elitism, which maintains the best solutions found in the search process. This ensures that the algorithm converges to the true Pareto-optimal front and avoids losing previously discovered optimal solutions.

- Crowding Distance: To maintain diversity in the population, NSGA-II uses a crowding distance (CD) mechanism. CD calculates the distance between neighboring solutions in the objective space, which is a measure of the density of solutions. CD enables the NSGA-II to select solutions that are optimal as well as well-distributed in the search space.
- Binary Tournament Selection: In this research, binary tournament selection (BTS) is used. BTS is mechanism to select individuals for mating based on their dominance rank and crowding distance. BTS helps in selecting individuals with better non-dominated ranks and higher CD by assigning a higher probability of selection.

The various steps of NSGA-II algorithm are as follows.

1. Initialize a random population (P) of candidate solutions.
2. Perform fast non-dominated sorting on P to classify solutions into different fronts.
3. Calculate the crowding distance for each solution within their respective fronts.
4. Select individuals for mating using binary tournament selection based on non-domination rank and CD.
5. Generate a new offspring population (Q) using genetic operators such as crossover and mutation.
6. Combine the parent and offspring populations (P $\cup$ Q) and perform fast non-dominated sorting.
7. Select the best solutions from the combined population based on non-domination rank and crowding distance until the desired population size is reached.
8. Repeat steps 4–7 for a predefined number of generations or until a stopping criterion is met.

2.3 MOGWO

The Multi-Objective Grey Wolf Optimizer (MOGWO) is a meta-heuristic optimization algorithm proposed by Mirjalili et al. in 2016 [16]. MOGWO is an extension of the single-objective Grey Wolf Optimizer (GWO) and aims to solve multi-objective optimization problems by simulating the social hierarchy and hunting behavior of grey wolves in nature. It provides an efficient and effective means to search for Pareto-optimal solutions in complex optimization problems with multiple conflicting objectives. The various key features of NSGA-II are as follows.

- Nature-inspired Optimization: MOGWO is inspired by the social behavior and hunting strategy of grey wolves in nature. It emulates their encircling, hunting, and attacking mechanisms, which helps guide the search towards optimal solutions in the problem space.
- Leader-based Hierarchical Structure: The algorithm uses a leader-based hierarchical structure, where the wolves are classified into three categories: alpha, beta, and delta. These leaders guide the rest of the pack (omega wolves) during the search process. This hierarchy facilitates better exploration and exploitation of the search space.
- Non-dominated Sorting and Grid-based Selection: MOGWO combines non-dominated sorting with a grid-based selection approach to maintain diversity and convergence towards the Pareto front. Non-dominated sorting classifies the solutions

into different fronts based on their level of domination. Grid-based selection divides the objective space into hypergrids and calculates the density of solutions in each grid, ensuring a well-distributed set of Pareto-optimal solutions.
- Adaptation of GWO Equations for Multi-objective Optimization: MOGWO adapts the original GWO equations to handle multiple objectives by utilizing the leaders' positions in a vectorized manner. This allows the algorithm to efficiently search for optimal solutions in problems with multiple conflicting objectives.

The various algorithmic steps of MOGWO are as follows.

1. Initialize a random population of candidate solutions (wolves).
2. Evaluate the objective function values for each solution.
3. Perform non-dominated sorting on the population to classify solutions into different fronts.
4. Use grid-based selection to calculate the grid density of each solution.
5. Identify the alpha, beta, and delta leaders based on their non-domination rank and grid density.
6. Update the positions of the wolves using the adapted GWO equations, considering the positions of the leaders.
7. Generate a new population by repeating steps 2–6 for a predefined number of iterations or until a stopping criterion is met.
8. Obtain the Pareto-optimal solutions from the final population.

3 Results and Discussion

3.1 Optimal Prediction with NSGA-II

Using Eqs. (1)–(3) as the objective functions, the energy consumption is minimized while maximizing the reaction conversion and green chemistry balance. A population size of 500 and an iteration limit of 100 generations have been implemented. The archive size for Pareto solutions is set to a maximum of 500.

Figure 1 illustrates the 3D Pareto front, representing the simultaneous minimization of energy consumption and maximization of reaction conversion and green chemistry balance. It is observed that the non-dominated solutions are in close proximity to one another, with distinct regions of discontinuity.

To further understand the effect of process parameters on the optimized responses, the NDS solutions that form the Pareto front in Fig. 1 are displayed as a parallel plot in Fig. 2. This visualization clearly illustrates the interaction between the process parameters and the responses. From the Fig., it is evident that within the NDS space, the energy consumption range is more extensive than those of reaction conversion and green chemistry balance.

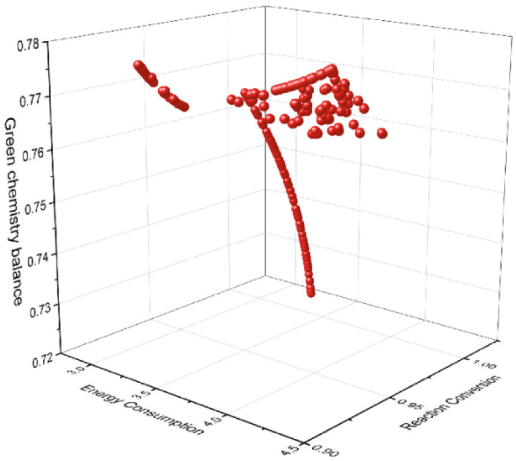

Fig. 1. 3D Pareto front generated by NSGA-II

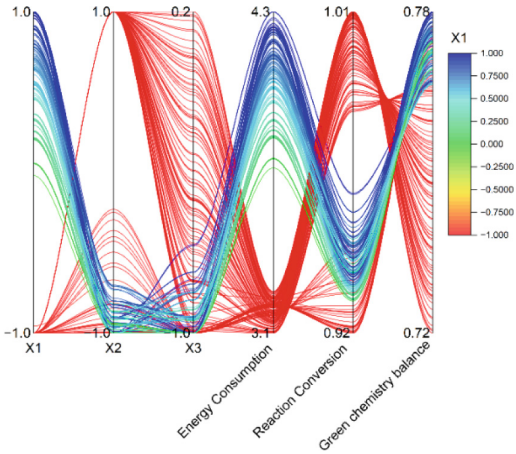

Fig. 2. Depiction of the interactions between process parameters and NSGA-II NDS solutions

3.2 Optimal Prediction with MOGWO

The test problem is addressed using the MOGWO algorithm, with the number of wolves set at 500 and the iteration limit at 100 cycles. To enable an unbiased comparison with the NSGA-II, the archive size in MOGWO is maintained at the same level as in NSGA-II, which is 500. The Pareto front generated by MOGWO is illustrated in Fig. 3, where it is observed that the MOGWO Pareto front appears less cluttered than that of NSGA-II. The MOGWO NDS solutions are further examined in Fig. 4, where a parallel plot is created to showcase the relationship between process parameters and responses. Generally, the trend observed aligns with that in the NSGA-II.

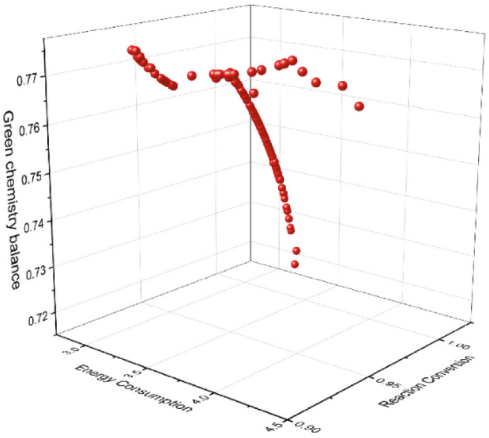

Fig. 3. 3D Pareto front generated by MOGWO

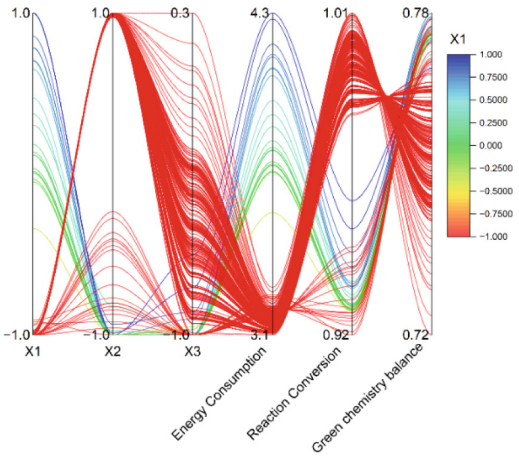

Fig. 4. Depiction of the interactions between process parameters and MOGWO NDS solutions

3.3 Comparative Analysis of NSGA-II and MOGWO Predicted Optimal Solutions

The computational time required by the NSGA-II and MOGWO are 67s and 53s, respectively. It is important to note that the simulations were conducted on a Dell Inspiron system featuring an Intel i7 processor, 24GB RAM, and a 500 GB SSD in a Windows environment. Consequently, MOGWO is found to be approximately 20% faster than NSGA-II.

The NDS solution sets of NSGA-II and MOGWO are visually compared using box plots, as depicted in Fig. 5. For each objective, clear distinctions between the NDS solutions generated by NSGA-II and MOGWO are evident. For example, in terms of energy consumption, the NSGA-II NDS solutions display a more uniform spread across the entire range, while MOGWO solutions are concentrated in the lower portion of

the range, with sparse and scarce solutions toward the upper region. Similarly, when comparing NSGA-II and MOGWO solutions for reaction conversion, Fig. 5 reveals distinct features for each algorithm. In the case of green chemistry balance, the NSGA-II NDS exhibit a long tail toward the lower portion of the range, whereas MOGWO solutions are evenly distributed across the entire range. In fact, the NDS solutions of MOGWO in the case of green chemistry balance closely follow a normal probability distribution.

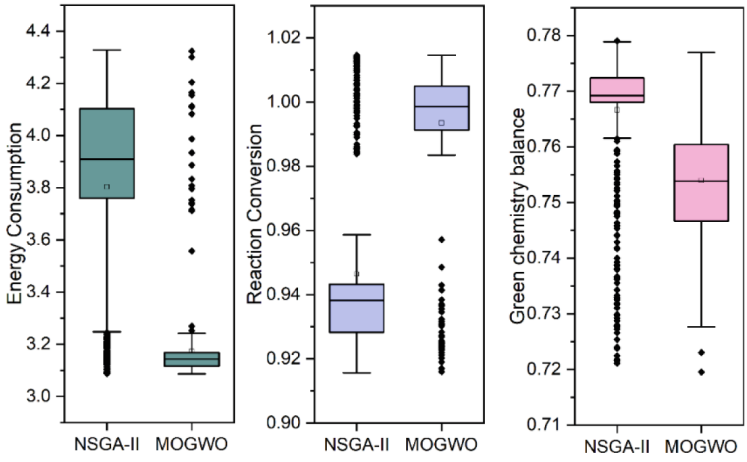

Fig. 5. Comparison of the NDS solution generated by NSGA-II and MOGWO

To make quantitative comparisons of the NDS solutions from NSGA-II and MOGWO, a multi-criteria decision-making method called COPRAS (Complex Proportional Assessment) is employed. COPRAS is an effective method for selecting a suitable compromise solution from a given set of alternatives. Four different weight-based scenarios are constructed using four weight allocation methods, namely mean weight method, entropy weight method, standard deviation weight method, and CRITIC weight method. A comprehensive discussion on COPRAS and the four weight allocation methods is beyond the scope of this article and can be found elsewhere [17, 18]. It is important to note that the combined Pareto fronts of both NSGA-II and MOGWO are treated as the alternatives, while energy consumption, reaction conversion, and green chemistry balance are considered as the criteria. Consequently, the initial decision matrix comprises 1000 alternatives and 3 criteria. The weights assigned to the three criteria by the four different weight allocation methods are listed in Table 1.

Table 2 presents the best compromise solution (BCS) among the combined total NDS, as determined by Mean weight-COPRAS, Entropy-COPRAS, Standard deviation-COPRAS, and CRITIC-COPRAS. Interestingly, for all four weight scenarios, the same set of solutions is identified as the BCS. However, due to varying weight factors in the different weight scenarios, distinct COPRAS Q-values are observed across the four scenarios. It is crucial to highlight that the BCS solution originates from the NDS generated by MOGWO.

Table 1. Weights assigned to the three criteria by different weight allocation methods

Weight Allocation Method	Energy Consumption	Reaction Conversion	Green Chemistry Balance
Mean weight	0.3333	0.3333	0.3333
Entropy	0.9101	0.0738	0.0162
Standard deviation	0.3873	0.3806	0.2321
CRITIC	0.3082	0.3385	0.3533

Table 2. Best compromise solution (BCS) by COPRAS for various weight scenarios

Weight Allocation Method	Energy Consumption	Reaction Conversion	Green Chemistry Balance	COPRAS Q-value	Predicted by algorithm
Mean weight	3.086	0.983467	0.766253	0.001045	MOGWO
Entropy	3.086	0.983467	0.766253	0.001105	MOGWO
Standard deviation	3.086	0.983467	0.766253	0.001051	MOGWO
CRITIC	3.086	0.983467	0.766253	0.001043	MOGWO

4 Conclusion

This study presents a comprehensive comparison between the NSGA-II and MOGWO algorithms for multi-objective optimization. The test case focuses on minimizing energy consumption while maximizing reaction conversion and green chemistry balance. The results show that MOGWO exhibits a less cluttered Pareto front as compared to NSGA-II. Moreover, MOGWO is seen to be approximately 20% faster than NSGA-II. Further the analysis of the NDS solution through box plots reveal that MOGWO NDS solutions are very distinct from the NSGA-II solutions.

Using COPRAS method, a quantitative comparison was made between the NDS solutions of NSGA-II and MOGWO for different weight scenarios. Interestingly, the same set of solutions was identified as the best compromise solution in all weight scenarios, which was in fact derived by the MOGWO NDS. This emphasizes the effectiveness and efficiency of the MOGWO algorithm.

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