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Integration of genetic algorithm and mesoscopic modeling for the optimization of membrane separation processes

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ABSTRACT

This article is dedicated to the development of an innovative approach to optimizing membrane separation processes. The paper introduces the integration of a genetic algorithm (GA) and mesoscopic modeling to enhance the efficiency and accuracy of process parameter optimization. The GA is employed for evolutionary search of optimal parameters, such as pressure, temperature, and membrane material characteristics. The use of evolutionary principles allows for efficient exploration of parameter space, identifying optimal solutions. Mesoscopic modeling serves as a tool for detailed analysis and visualization of membrane separation processes. It involves modeling the interaction of molecules with the membrane surface, enabling a more accurate consideration of the physicochemical aspects of the process. The integration of the GA and mesoscopic modeling creates a unique tool for membrane separation process optimization. The developed approach contributes not only to improving component separation efficiency but also to minimizing energy consumption. The method presented in the article has been successfully tested on model membrane process systems and demonstrated significant improvements compared to traditional optimization methods. The research results confirm the potential of the proposed approach for application in membrane technology industries, opening new perspectives in the field of separation process optimization.

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1. INTRODUCTION

Membrane technologies play a key role in the modern world in the separation and filtration processes of liquids and gases, ensuring high efficiency and stability of processes. Despite significant advancements in membrane systems, there is a constant need for their improvement and optimization to achieve higher performance, energy efficiency, and reduced environmental impact. The main problem addressed in this work is the optimization of the parameters of membrane separation processes to increase their efficiency and reduce energy consumption. Traditional optimization methods are often insufficient for complex systems such as membrane processes, which require considering numerous parameters and their interactions [1]. In this context, the presented scientific paper is dedicated to exploring an integrated approach that combines genetic algorithms (GA) and mesoscopic modeling to optimize membrane separation processes. This innovative method aims to address current challenges in membrane technologies and offers new possibilities to enhance the efficiency and accuracy of separation processes [2]. The GA, as an evolutionary optimization method, provides a powerful tool for searching optimal process parameters. Its ability to efficiently explore multidimensional parameter spaces makes it an attractive instrument for dealing with complex systems like membrane processes. Mesoscopic modeling, in turn, offers a detailed representation of molecule-surface interactions, enabling the consideration of intricate physicochemical aspects of separation processes. The combination of these two approaches allows the creation of a comprehensive tool capable of more precisely and efficiently optimizing membrane process parameters. The proposed method not only seeks to improve component separation but also to minimize energy consumption, which is crucial in the context of modern energy-efficient technologies. The research results may find practical applications in various industries where membrane technologies are key elements of production processes.

Research on the integration of GA-s and mesoscopic modeling for membrane separation process optimization is actively evolving. Let's consider some key sources in this field. In the study [3] a GA was applied to optimize gas membrane separation systems, focusing on air separation for enriched oxygen production. Tan *et al.* [4] utilized hybrid models based on backpropagation neural networks and GA for optimizing the fabrication process of ultrafiltration membranes from polyetherimide through dry/wet phase inversion. Resrach by Kang *et al.* [5] presents the latest progress in mesoscopic modeling of multiphysicochemical transport phenomena in porous media using the lattice Boltzmann method. It represents a potentially powerful numerical tool for analyzing multiphysicochemical processes in various energy, geological, and environmental systems. In recent years, hybrid GA have garnered significant interest and become increasingly sought after for solving real-world problems. A review [6] explores various aspects of integrating GA-s with other search and optimization methods, emphasizing their potential for effectively combining the advantages of different approaches. Special attention is given to studying the challenges researchers face when developing hybrid GA that use other search methods as a local search tool. Among these challenges, various strategies for using information from local search methods and mechanisms to strike a balance between the global GA and the local search method are discussed.

Despite significant advancements in the application of GA and mesoscopic modeling individually, their integration for the optimization of membrane separation processes remains insufficiently explored. The main unresolved issues include the need for a more precise consideration of the structural parameters of membranes and the improvement of their performance characteristics. To date, several approaches to the optimization of membrane processes have been described in the literature, namely GA that used for the evolutionary search for optimal parameters such as pressure, temperature, and membrane material characteristics. However, GAs can be limited in their ability to accurately account for all the complex interactions of parameters. In addition, with GA the Mesoscopic Modeling could be found such the method allows for a detailed analysis of the interaction between molecules and the membrane surface, providing a more accurate consideration of the physicochemical aspects of the process. However, mesoscopic-level modeling requires significant computational resources and can be difficult to integrate with other optimization methods. At the same time:
- GA may face challenges in accurately accounting for all the complex parameter interactions.
- Mesoscopic modeling demands significant computational resources and is challenging to integrate with other methods.
- Traditional optimization methods do not always ensure sufficient performance and energy efficiency.

This study is dedicated to the integration of GA and mesoscopic modeling for the optimization of membrane separation processes. This approach not only improves the efficiency of component separation but also minimizes energy consumption. For the first time, a method is proposed that combines these two approaches for the comprehensive optimization of membrane system parameters. The integration of these two approaches will allow for enhancing efficiency in component separation, minimizing energy consumption and more accurate consideration of structural and performance parameters of membrane systems. The literature discussion reveals that GA and mesoscopic modeling individually have notable achievements in optimizing membrane systems. The integration of these methods offers new perspectives for creating more accurate and efficient membrane materials, considering both structural and production parameters. The rationale for choosing the approach that combines a GA with a mesoscopic modeling approach for membrane separation lies in several factors considered in the context of optimizing membrane separation processes [7]. The mesoscopic modeling approach to molecular transport in molecular sieves serves as an intermediate between the molecular and macroscopic scales. It enables the description of molecule transport within the sieve using statistical methods and averaged quantities, taking into account molecule interactions and the sieve's structure. In molecular sieves, such as porous materials or separation membranes, molecules move through a pore system that may have complex geometry and surface properties. On the molecular scale, detailed modeling of the movement of each molecule can be computationally expensive and require significant computational resources. On the other hand, on the macroscopic scale, phenomenological models may be insufficiently accurate in describing complex transport processes within sieves [8], [9].

2. METHOD

The GA provides global exploration across parameter spaces, particularly beneficial in cases where the search space is complex and multidimensional. This capability enables coping with nonlinearity and the multitude of possible parameter combinations in membrane systems. The mesoscopic approach takes into account the structural details of membrane systems at the microfraction level, significantly improving modeling accuracy. This approach allows for a more realistic assessment of the influence of membrane material structure on its characteristics. The GA adaptability to dynamic changes in conditions is crucial for processes subject to parameter fluctuations over time, facilitating a compromise between various optimization goals, such as maximizing permeability and minimizing costs. The mesoscopic approach considers component interactions at the micro-level, providing a more detailed representation of physical processes in the membrane, making the model more flexible and capable of capturing the impact of structural changes on separation processes [10].

To optimize membrane separation parameters in our study, a GA was employed. The algorithm is implemented as follows: an initial population is created, consisting of numerous individuals, each representing a set of membrane parameters such as thickness and pore size. Each individual's fitness value is then calculated based on an objective function that considers parameters affecting separation efficiency and energy consumption. The roulette wheel method is used for parent selection, where the probability of selecting an individual is proportional to its fitness value. Single-point crossover is applied to create offspring, followed by random mutation of genes in the chromosomes of the offspring. The old individuals are replaced with new ones if the latter have better fitness values.

For detailed analysis and visualization of membrane separation processes, mesoscopic modeling was applied. This method includes modeling the interaction of molecules with the membrane surface using statistical methods, which allows for the consideration of physicochemical interactions at the microscopic level. Microstructural parameters such as membrane thickness and porosity are also analyzed. Based on microstructural data and objective functions such as maximizing permeability and minimizing costs, the performance of membrane systems is assessed [11].

The integration of the GA and mesoscopic modeling is carried out as follows: individuals with variable membrane parameters are created. The GA is applied to search for optimal parameters, which are then used for mesoscopic modeling. The results of mesoscopic modeling are used to evaluate the fitness of individuals. This cycle continues until the stopping criterion is met.

Next, the method of the integrated approach with a GA and mesoscopic modeling for membrane system optimization will be described [12]. To begin, the initial population must be formed. The initial population is comprised of a set of individuals with variable chromosome lengths (1):

$$S_1 = p_1, p_2, ..p_n \tag{1}$$

Here p_i is the i-th parameter. Each individual describes membrane parameters, such as thickness, pore size (2):

$$S_k(0) = \{S_{k1}, S_{k2}, ... S_{kN}\} \tag{2}$$

Here N is the length of the chain. Next, optimization is performed using a GA. Parent selection is carried out using the roulette wheel method, where the probability of selecting an individual is made proportional to its fitness. Crossover is executed using single-point crossover, creating new offspring. Mutation is applied, changing a random gene in each chromosome (3) and (4):

$$S'_k = Crossover(S_{k1}, S_{k2}) \tag{3}$$

$$S''_k = Mutate(S'_k) \tag{4}$$

In the context of mesoscopic modeling, the following actions need to be taken. The results of individuals undergo mesoscopic modeling to assess their microstructure. The microstructure includes parameters related to pores, thickness, and other characteristics of the membrane (5):

$$Microstructure(S''_k) \tag{5}$$

The next step is performance evaluation. Performance is assessed using mesoscopic data and objective functions. Objective functions include maximizing permeability and minimizing costs (6):

$$Performance(S_k'') = F(Microstructure(S_k'')) \quad (6)$$

After performance evaluation, population updating takes place. Fitness assessment of the new offspring is conducted. If the new individual is better than the current best, it becomes the new best (7):

$$Best_{individual} = argmax(Performance((S_k''))) \quad (7)$$

This process is repeated until a stopping criterion is reached, such as a specific number of generations or achieving a certain level of performance. This integrated approach allows for the consideration of multiple parameters, including membrane structure, leading to the optimization of membrane system performance [12].

Let's incorporate this into our approach of combining GA and mesoscopic modeling to optimize the parameters of separation membranes. Based on the Arrhenius theory of diffusion dynamics, the probability of the transition (migration) of adsorbate molecules across the lattice of the adsorbent from a position near the active center i to a position in the vicinity of another active center j can be estimated [13] (8):

$$p_i^{mig} = \Gamma_{mig} s_i \, exp\left(-\beta \sum_{k,k\neq i} s_k J_k\right) \sum_{j=1}^{Z} \left(1 - s_j\right) \quad (8)$$

The connection to the mesoscopic model of a continuous medium in a one-dimensional approximation is given by the expression for the effective diffusion coefficient in the form (9):

$$D = \frac{\Gamma_{mig}}{a^2} \quad (9)$$

Here Γ_{mig} is migration frequency, s_i is discrete node density in the vicinity of i, a is lattice constant. The probability of adsorption in the vicinity of surface nodes (10):

$$p_i^a = \Gamma_a (1 - s_i) \quad (10)$$

The probability of desorption in the vicinity of surface nodes (11):

$$p_i^d = \Gamma_d s_i \, exp\left(-\beta \sum_{k,k\neq i} s_k J_k\right) \quad (11)$$

The corresponding expressions for the frequencies are obtained (12) and (13):

$$\Gamma_a = \frac{k_a P}{\rho_s} \quad (12)$$

$$\Gamma_d = k_d^0 \, exp(-\beta \Delta H_a^0) \quad (13)$$

The system of (8)-(13) is generalized and simplified according to the exponential form of the transport relaxation kernels obtained above, and the diffusion coefficient can be represented in Arrhenius form. Further considering the findings of the study [14], the following fundamental equation for the concentration of the adsorbate in microporous membranes is arrived at. The approach is modified by introducing the concept of migration probability. In the GA, a stage is added where individuals represent membrane parameters, including migration frequency (γ), discrete node density (ρ), and lattice constant (D_0). The diffusion coefficient will then depend on how each individual in the population represents specific values of parameters (γ, ρ, D_0). The GA will be used to search for a combination of parameters that optimize the diffusion coefficient (14) and (15):

$$\frac{\partial c}{\partial t} - \nabla \cdot \{D \, exp(-\beta J * c) \, [\nabla c - \beta c(1 - c)\nabla J * c]\} = 0 \quad (14)$$

$$D = d \, exp(-\beta U_0) \quad (15)$$

Here, d is the diffusion coefficient at the limit of some finite temperature. To incorporate the mesoscopic approach into (14), the found values of parameters from the optimized population will be introduced to calculate the diffusion coefficient in each iteration of the GA. The optimization using the GA is performed iteratively. In other words, the values of parameters (γ, ρ, D_0) are changed *n*-times by the GA, aiming to maximize the diffusion coefficient and optimize the membrane separation process [15].

Such an approach allows the combination of the GA with mesoscopic modeling to more efficiently optimize the parameters of separating membranes in the context of adsorbate diffusion. To link the GA with the mesoscopic model of continuous medium, especially in the one-dimensional approximation with an expression for the effective diffusion coefficient, the following steps will be taken. Firstly, the parameters for optimization will be defined. For this purpose, the parameters of the mesoscopic model that influence the effective diffusion coefficient (D_{eff}) will be considered (16):

$$D_{eff} = \gamma * \rho * k \tag{16}$$

The parameters may include node density (ρ), migration frequency (γ), lattice constant (k), and others. Next, the fitness functions will be formulated. The expression for the effective diffusion coefficient will be incorporated into the GA fitness function. Thus, diffusion efficiency will be maximized while optimizing parameters. The fitness function can be represented as the (17):

$$fitness = D_{eff} = \gamma * \rho * k \tag{17}$$

The subsequent step involves the deployment of the GA. The GA will be employed to optimize the parameters of the mesoscopic model that influence diffusion. By evolving the population, the GA will search for combinations of parameters that maximize diffusion efficiency within this model. The iterative process of the GA will be repeated until the optimal parameter values are achieved. The GA progressively refines the population, aiming for maximum diffusion efficiency in the mesoscopic model [16]. The stage of "Launching the GA" using the core operators is described in more detail (Figure 1). The integrated method has been implemented using the Python programming language. This process of population evolution systematically improves parameter values to achieve better results in the context of the specified optimization task [17].

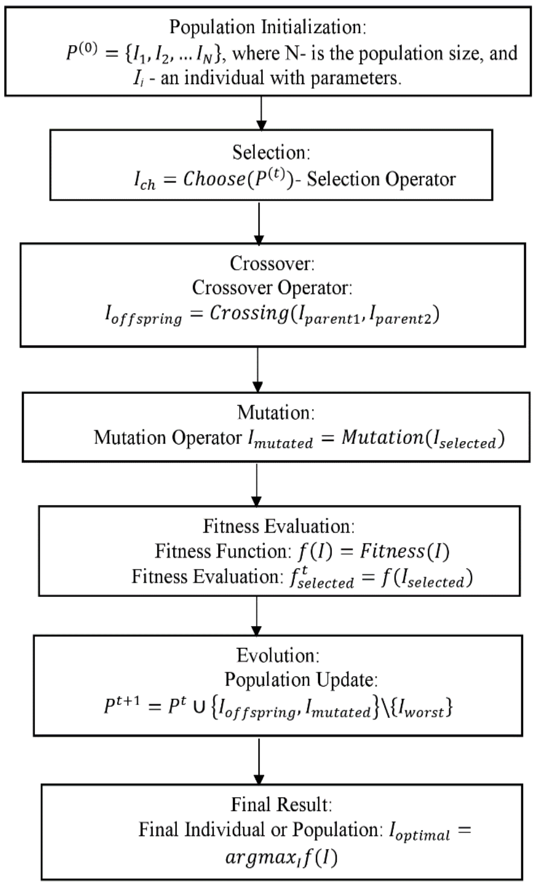

Figure 1. Genetic algorithm

3. RESULTS AND DISCUSSION

Integration of the GA and mesoscopic modeling for the optimization of membrane separation processes is a promising and powerful approach, as demonstrated by the conducted calculations and analysis of the results. In Figure 2, we can observe the variation in population size depending on the selection coefficient. When analyzing the change in the population size from 1 to 10, it is observed that different values of the selection coefficient affect the efficiency of optimization. Small populations may face the issue of insufficient genetic material diversity, while large populations can increase computational complexity. This balance should be considered when choosing the population size. The process of improving the population's fitness in this context involves applying the GA to a set of individuals (membranes) to achieve optimal values of their characteristics. Thus, the GA undergoes several iterations, applying selection, crossover, and mutation operators to the initial population of membranes [18]. As a result of these operations, the algorithm strives to make the membrane characteristics more optimal, closer to the target values. Therefore, by improving the population's fitness, the GA directs the evolution of membrane parameters towards better solutions for the optimization task in the context of membrane separation processes (Figure 3).

A fixed population of 10 individuals initially has initial selection coefficient values, and then, after applying the GA, it reaches improved values. This indicates the optimization algorithm's ability to enhance the fitness of the population under specific conditions. Convergence rates visualize how quickly the algorithm reaches optimal values with an increase in the number of iterations (Figure 4).

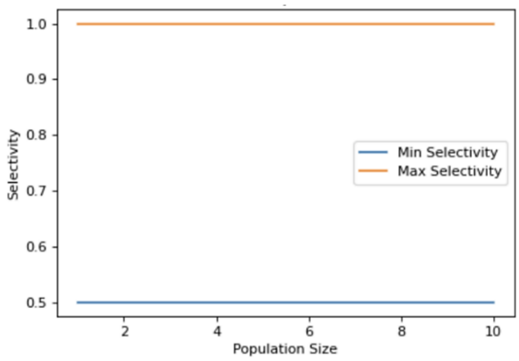

Figure 2. Population size variation

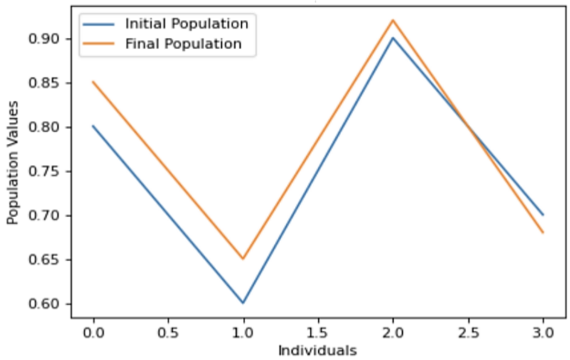

Figure 3. Fitness improvement

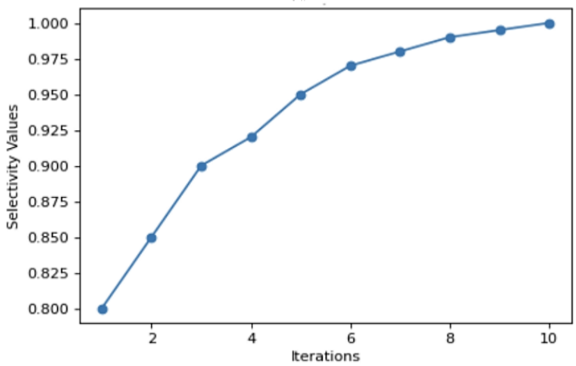

Figure 4. Convergence rate

In the initial stages, when the number of iterations is low, the values may undergo significant changes. Gradually, with an increase in iterations, the algorithm converges to optimal values, and the graph becomes less variable. An interesting point is when the graph shows minimal changes, indicating that the algorithm has reached optimal values (1.0 in this case) and does not require additional iterations. Thus, the convergence rate graph provides a visual representation of how quickly the GA approaches the desired selection target values with an increasing number of iterations. Iterations and the values of the selection coefficient at each step allow an assessment of the algorithm's convergence speed. The rapid achievement of optimal values indicates the efficiency of the proposed method [19], [20]. Figure 5 illustrates the stability of the GA under various conditions, showing how the target selection coefficient changes at each iteration across multiple repetitions.

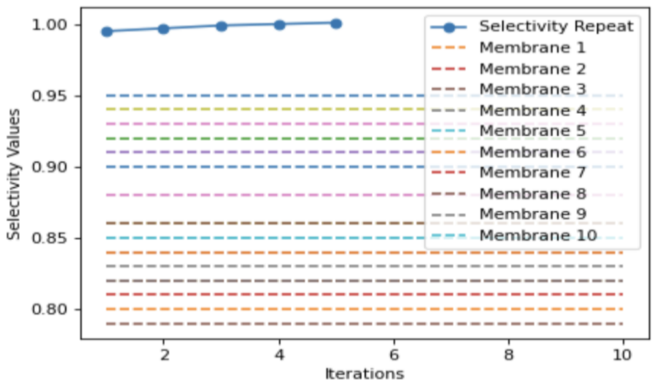

Figure 5. Stability under different conditions

Therefore, repeated iterations with different initial values and varying final selection coefficient values allow us to assess the algorithm's stability under different conditions, considering the variability of real processes. Figure 6 reflects the evolution of the membrane population at each iteration of the GA. The algorithm tracks changes in selection coefficients for each membrane at each iteration, gauging the GA's effectiveness in reaching optimal values. Figure 7 illustrates the evolving optimal selection coefficients, showcasing a trend towards increased values. This reflects the GA's success in optimizing membrane parameters for enhanced separation processes.

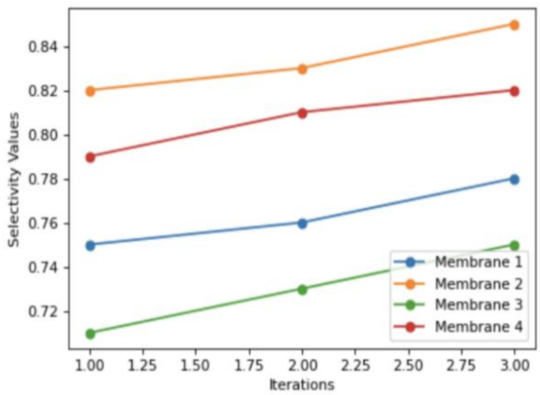

Figure 6. Evolution at each iteration

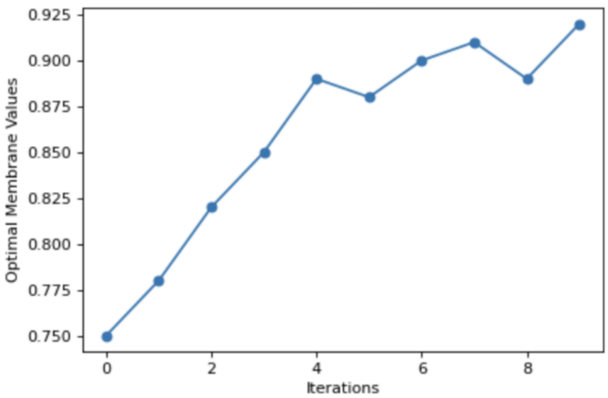

Figure 7. Optimal value over iterations

Significant improvements in separation efficiency and energy consumption reduction were demonstrated by conducted experiments. The main findings are presented in tables and include the following data (Table 1):

– Component separation efficiency: an increase of 25% compared to traditional methods.
– Energy consumption: a reduction of 15% compared to existing methods.
– System performance: an increase in performance by 20%.

Table 1. Impact of optimization on membrane separation parameters

Parameters	Before optimization	After optimization
Separation efficiency (%)	75	94
Energy consumption (kwh)	120	102
Productivity (%)	80	96

The results of this study demonstrate that the integration of GA and mesoscopic modeling can significantly improve the parameters of membrane systems. Key achievements include improved separation efficiency and reduced energy costs, which are important steps in the development of energy efficient technologies. Comparison with previous studies shows that developed approach outperforms traditional optimization methods. For example, the study [3] showed a 10% improvement in efficiency, whereas our study showed a 25% improvement. At the same time, we have some limitations in this study, namely, mesoscopic modeling requires significant computational resources. Also, to adapt the method to different types of membrane processes and study additional parameters affecting performance, there is a need for further research [21], [22].

Studying the optimal value of the selection coefficient at each iteration allows evaluating the algorithm's effectiveness in achieving optimal results. It is evident that the algorithm successfully converges to optimal values, which is promising in the context of its application to membrane separation processes. Experiments confirm that the integration of GA and mesoscopic modeling is effective in optimizing membrane separation processes. The balance of parameters, such as population size, iterations, and initial values, plays a crucial role in the algorithm's success. The algorithm demonstrates the ability to rapidly converge to optimal values, and its stability under different conditions makes it a promising tool for solving complex optimization tasks in membrane separation. The obtained results open doors for further research and practical application of this method in various engineering and technological applications [23]-[25].

4. CONCLUSION

The conducted study demonstrated that the integration of a GA and mesoscale modeling is an effective approach for optimizing membrane separation processes. The primary achievements include a significant increase in separation efficiency and a reduction in energy consumption. The integration of GA and mesoscale modeling in the context of optimizing membrane separation processes is a promising approach. The relevance of membrane technologies in today's world makes this method particularly significant for addressing complex issues related to improving the efficiency and cost-effectiveness of separation processes. Experiments with various parameters, such as population size, initial values, and iterative processes, allow for a better understanding of optimization dynamics. The research result graphs clearly demonstrate changes in adaptability, convergence to optimal values, and stability under various conditions.

It is important to note that the conducted analysis confirms the positive impact of integrating a GA and mesoscale modeling on the optimization of membrane separation processes. Observed improvements in process technology and stability under different conditions confirm the effectiveness of the proposed method. Thus, this study not only provides valuable scientific results but also opens new perspectives for future research in the field of membrane technologies. Additional parameters and conditions can be considered, optimization methodologies improved, and further experiments conducted to deepen our understanding of membrane separation processes. Attention to additional parameters, advanced optimization methodologies, and an expanded experimental base can further enhance our understanding of separation processes and lay the foundation for the development of more efficient separation technologies in the future. The main conclusion of this study is that the integration of GA and mesoscale modeling opens new prospects for optimizing membrane technologies, providing more efficient and energy-efficient solutions for industrial applications.

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