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Multi-Objective Optimization Pressure Swing Adsorption for Small-Scale Nitrogen Production Based on Meta-Heuristic Method

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ABSTRACT

Background: The global increase in fertilizer prices and weakening food security highlight the urgency of decentralized green ammonia production. The main challenge in small-scale ammonia systems is achieving stable, high-quality nitrogen production. Although, Pressure Swing Adsorption (PSA) capable of addressing this challenge, it requires optimization due to complex parameter interactions and energy requirements. Existing studies have mostly focused on large scale or single-objective optimization, with few exploring multi-objective approaches to small-scale nitrogen purification.
Aims and Method: This study aims to optimize nitrogen purity, achieve a target flow rate and reduce energy consumption in a PSA system using zeolite 13X. A meta-heuristic optimization framework integrating Genetic Algorithm (GA) and Particle Swarm Optimization (PSO) is developed. The optimization involves key variables such as adsorption–desorption pressures, cycle times, bed dimensions, and adsorbent mass. Sensitivity analysis and monte carlo simulation were applied to evaluate parameter influence and ensure operational robustness.
Results: GA-PSO optimization method result achieved a high nitrogen product flow rate (≈298kmol/h), high purity (≈99%), while maintaining energy consumption level significantly lower than conventional methods (≈120$/h). Furthermore, sensitivity analysis using ANN revealed that bed length, desorption time, and pressure conditions exhibit the highest influence on PSA performance.

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1. Introduction

The synthesis of ammonia (NH_3) has become one of the most crucial sources of nitrogen supply in the agricultural industry, particularly for fertilizer continent for plant growth. The Haber-Bosch (HB) process is used globally for the mass production of NH_3, with a worldwide production capacity of approximately 188 million metric tonnes and growth rate of 1.54% annually (Liu *et al*., 2023). Despite the increasing production growth rate, agricultural challenges persist in rural areas. The price surge of fertilizer increased by 70% has led to decreased agricultural productivity, negatively impacting a national food security (Bora *et al*., 2024). The main factor is the centralized ammonia production, which often requires transportation infrastructure to be allowed one or another component of the process that became one of the problems as it increases costs and environmental risks. Price increases in fertilizers can be suppressed by the decentralized NH_3 production method. However, building a small-scale NH_3 industry requires calculation and optimization of process parameters to a smaller scale.

Capital cost of equipment, periodic and expensive maintenance are an additional reason to consider the best method and parameter for small-scale production. Membrane permeation is suitable at small scale, but the low purity of nitrogen obtained makes this alternative unfeasible when other options are available. Low N_2 purity is fatal because gas streams such as O_2 that are carried can poison the catalyst in the NH_3 synthesis process (Folke *et al*., 2020). Thus, Pressure Swing Adsorption (PSA) is the most promising nitrogen production method because it is able to produce high purity N_2 and is economical in terms of energy. Other advantages such as low operating system, compact design, and environmental-friendly operation make it suitable for N_2 system in small-scale NH_3 industry. PSA obtains N_2 by separating the environmental air content which is composed of 78% nitrogen, 21% oxygen, 1% argon and other gases. The N_2 production rate required in the small-scale NH_3 industry is 298 kmol/h with a purity level that must be maintained in the range of 98-99.9% (Spatolisano & Pellegrini, 2023). Producing high-purity N_2 in the quantity required for the small-scale NH_3 industry requires a lot of energy for the gas adsorption process. Therefore, this optimization research is critical because achieving reliable high-purity nitrogen at an energy-efficient operating point directly determines the feasibility, sustainability, and economic viability of decentralized small-scale ammonia production systems.

Conventional optimization methods can be performed but have long computation time and unstable convergence, thus triggering optimization failure. Along with the development of computing technology, meta-heuristic algorithms were developed to solve problems in the field of multi-objective optimization. In previous research, Tan *et al*. (2024) applied meta-heuristic optimization method to find the optimal combination of parameters of separation technologies such as hydrocyclones. With result, meta-heuristic can maximize separation efficiency while minimizing pressure loss. Ruan *et al.* (2023) also in their study combined 3 heuristic methods in optimizing the energy efficiency of the separation process for the synthesis of polyolefin elastomers. The proposed optimization method can reduce TAC and CO_2 emissions simultaneously, while maintaining good controllability. From some of the above studies, it can be concluded that the meta-heuristic algorithm is suitable for the application of multi-objective optimization in complex separation systems with conflicting objectives while meeting any given constraints.

Limited attention has been given to small-scale decentralized green NH_3 production and its integration of meta-heuristic, especially in achieving high purity N_2 at the target flow rate simultaneously optimizing the energy demand of the PSA system. Previous studies predominantly focused on single-objective optimization or large-scale units, without addressing the multi-objective trade-offs required for small-scale applications. Moreover, most works neglected cross-validation between optimization results and physical adsorption behavior, leaving a gap between computational outcomes and process realism. This study fills this gap by developing a multi-objective optimization framework using combined Genetic Algorithm (GA)–Particle Swarm Optimization (PSO) algorithms for PSA-based nitrogen production. Monte Carlo validation ensures result consistent with real operating scenarios, while Artificial Neural Network (ANN) based sensitivity analysis identifies variable influence. The objective of this integrated research framework is to ensure that the PSA

system can deliver the required nitrogen flow rate for small-scale ammonia production with high product purity, while simultaneously minimizing energy consumption and maintaining consistency with real operational performance.

2. Methods

2.1 Model description and limitations

In this study, two-bed PSA system configuration is employed. Operating based on four-step cycle to ensure continuous N_2 production to reach the quantity and purity of product while optimizing energy consumption. The process flow of the PSA system from environmental air to nitrogen product can be seen in Figure 1. Variables that affect the effectiveness of the PSA separation process include the following, adsorption pressure (P_{ads}), desorption pressure (P_{des}), adsorption time (t_{ads}), desorption time (t_{des}), purge time (t_{purge}), bed length (l), bed diameter (d), and adsorbent mass ($m_{adsorbent}$) (Bulfin *et al.*, 2021). The PSA systems utilize a fixed-bed adsorption column, in which O_2 and Ar are selectively adsorbed onto the nanoporous material under high pressure. Zeolite 13X is considered the most suitable adsorbent type in separating N_2 because it has a smaller quadrupole moment so that O_2 is more easily adsorbed than N_2.

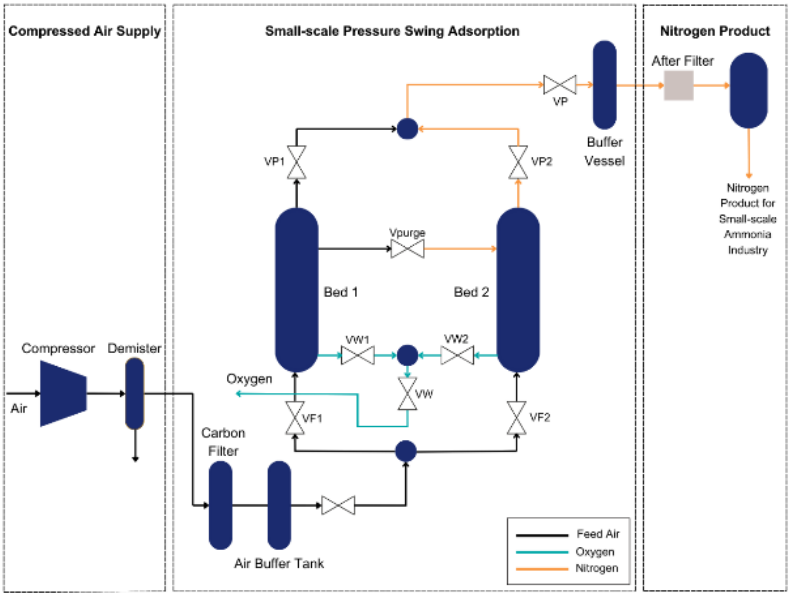

Figure 1. Flowsheet of PSA nitrogen production distribution system for small-scale ammonia industry.

Although meta-heuristic optimization has been widely applied to various separation technologies (Gharibi *et al.*, 2024), its integration into small-scale PSA configurations for decentralized ammonia production has not been adequately explored. In this study, the PSA model is developed by considering several assumptions in simplifying the complexity of the real system to improve the accuracy and efficiency of calculations in the optimization process using the Meta-Heuristic Algorithm (MHA). Therefore, the assumptions adopted in this PSA model are specifically designed to close this research gap by enabling the MHA to evaluate multi-objective interactions under realistic small-scale operating conditions such as:

a. the adsorption properties of adsorbent, void fraction, and gas viscosity remain unchanged;
b. the gas is assumed to be an ideal gas with a uniform flow profile.
c. inlet gas in the form of air mixture with fixed composition;
d. compressor and vacuum pump energy efficiency set constant;
e. plug flow with axial dispersion occurs;
f. thermal equilibrium exists between the gas phase and the adsorbent;

2.2 Baseline parameter

The process flow diagram of the PSA system, as presented in Figure 1, serves as the basis for defining the operational parameters used in the meta-heuristic optimization. Literature and mathematical model approaches are carried out to find the optimal range of variable values to facilitate meta-heuristic calculations in achieving the target criteria, as shown in Table 1 (Spatolisano & Pellegrini, 2023). Additionally, a comparison of parameters used in different nitrogen separators employing PSA technology is presented in Table 2. This comparison includes adsorption and desorption conditions, cycle times, adsorbent types, and resulting nitrogen purity and flow rates from various studies. The parameter range in Table 3 is used in MHA which is further calculated in the objective function. The range used here was selected based on thermodynamic considerations and the proportional benefits obtained in terms of adsorption rate and energy consumption for small-scale NH_3 industry

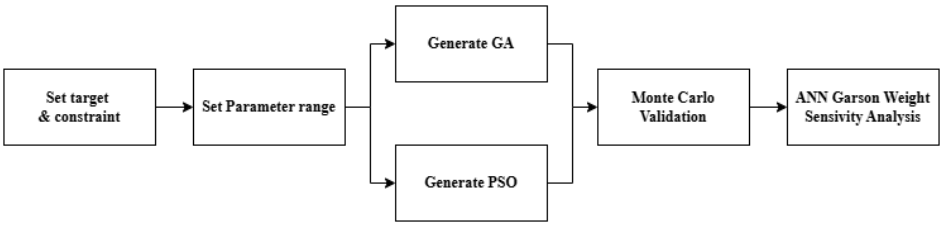

Figure 2. Research Method Framework

Table 1. Target criteria for Meta-Heuristic Optimization

Variable	Target
$\dot{F}_{N_2}$	298 kmol/h
Purity	98-99.9%
Energy	As low as possible

Table 2. Comparison of parameters in different nitrogen separators using PSA

Method	Numerical	Analytic	Numerical
Author	Benkirane et al.	Aly et al.	Bulfin et al.
Feed gas mole fraction	78% N_2, 21% O_2	88% N_2, 12% CO_2	99% N_2, 1% O_2
Adsorption pressure (bar)	10	1	20
Desorption pressure (bar)	1	0.2	0.005
Adsorption time (s)	40	70	
Desorption time (s)	30	60	46080 (1 cycle)
Purge time (s)	30	90	
Energy consumption ($/h)	150-270	142.38	8.18
Bed length (m)	2	1	0.5
Bed diameter (m)	0.5	0.324	0.5
Adsorbent mass (kg)	471.182	46.7	855
Adsorbent	Zeolite-5A	Zeolite K(23)Y	Unspecified
Purity (%)	96	90	99.999%
Product flow rate (kmol/h)	131.233	91.346	44.233

Table 3. Meta-heuristic parameters setting

Variables	Upper bound	Lower bound	Unit
Adsorption pressure (P_{ads})	4	20.5	bar
Desorption pressure (P_{des})	0.1	1	bar
Adsorption time (t_{ads})	300	900	s

Desorption time (t_{des})	120	300	s
Purge time (t_{purge})	60	120	s
Bed length (l_{bed})	1	3	m
Bed diameter (d_{bed})	0.3	1	m
Adsorbent mass ($m_{adsorbent}$)	10	100	kg

Mathematical models are used to define the objective function in the heuristic method and find suitable parameter range settings for small-scale PSA systems. Algebraic equations of substantially lower order are employed to reformulate the PDE, resulting in much simpler representation for PSA models and enhancing the computational efficiency of meta-heuristic optimization problems. Cycle time (t_{cycle}) can be calculated using Eq. (1).

$$t_{cycle} = t_{ads} + t_{des} + t_{purge} \quad (1)$$

where, t_{ads} represent the adsorption time, t_{des} is the desorption time and t_{purge} as the cleaning cycle time. Next, the variable volume of the adsorbent bed is calculated to determine how much space is used for sorbate gas absorption media. In calculating the volume of the cylinder can use Eq. (2). Eq. (3) is used to calculate the upper and lower cross-sectional areas of the bed. The total volume of the bed is calculated using Eq. (4).

$$V_1 = \frac{\pi.d^2.l}{4} \quad (2)$$

$$V_2 = 0.0847d^3 \quad (3)$$

$$V_{bed} = V_1 + 2.V_2 \quad (4)$$

P_r refers to the performance of the PSA in absorbing sorbate gas (kg/m^3.h or kmol/m^3.h) from the air. The amount of sorbate gas adsorbed is summarized and can be calculated in Eq. (5). Where madsorbent is the mass of zeolite 13X adsorbent, MW_{O2} is the molecular weight of O_2, and ε_b is the void in the bed (usually around 0.4).

$$P_r = \frac{q.m_{adsorbent}.MW_{O_2}.10^{-3}}{V_{bed}.(1-\varepsilon_b).t_{cycle}} \quad (5)$$

$$P = F - P_r \quad (6)$$

$$\text{Purity} = \frac{F - \left(\frac{P_{des}}{P_{ads}}\right).P}{F-P} \quad (7)$$

$$\dot{F}_{N_2} = F\ .\ Purity \quad (8)$$

The purity of N_2 product can be calculated using Eq. (7). Finally, Eq. (8) is used to calculate the flow rate value of N_2 product. Eq. (1)-(8) are the equations used to define the objective function in the MHA used in this study.

2.3 Meta-heuristic algorithm

Meta-heuristic algorithms have been developed over the past few decades to address variable optimization problems. Basically, meta-heuristic is a combination of several heuristic approaches to cover the shortcomings of a heuristic method. Single heuristic methods have shortcomings such as being vulnerable to being trapped in local solutions and there is no guarantee that the results obtained are optimal. MHA are able to explore a wider solution space and avoid local traps (Lu *et al*., 2024). MHA is suitable for problems involving several complex variables that have linear, non-linear, discrete or continuous values such as in PSA systems. This research combines two modeling heuristic GA and PSO to find the globally optimal solution.

2.4 Genetic algorithm (GA)

GA is considered a non-deterministic problem solver inspired by genetic variation and natural selection. The double vector population uses a representative of each individual named, 0 and 1 as the genotype part. In double vector each chromosome is represented as: [P_{ads}, P_{des}, t_{ads}, t_{des}, t_{purge}, l, d,

$m_{adsorbent}$]. Furthermore, to achieve the optimal solution is accomplished using some basic elements such as population, crossover and mutation involving chromosomes as a representation of individuals. The selection of their values is crucial as they can significantly affect the ability and total iteration time. The selection of individuals that have high fitness values is used as the parent for each parameter. Parent will experience reproduction of each variable and the selected pair of individuals will be performed crossover and mutation functions (Wu *et al*., 2022). The crossover rate used in this study is 0.8 with the aim that the GA has more population diversity so that the exploration of solutions increases. After the crossover process, the mutation operation is performed to prevent getting stuck in a local solution. The mutation value used is 0.1. The reproduction stage is repeated in the new generation, and the optimization process continues until it finds a solution with the best fitness value. The process flow of optimizing PSA with GA is shown in Figure 3.

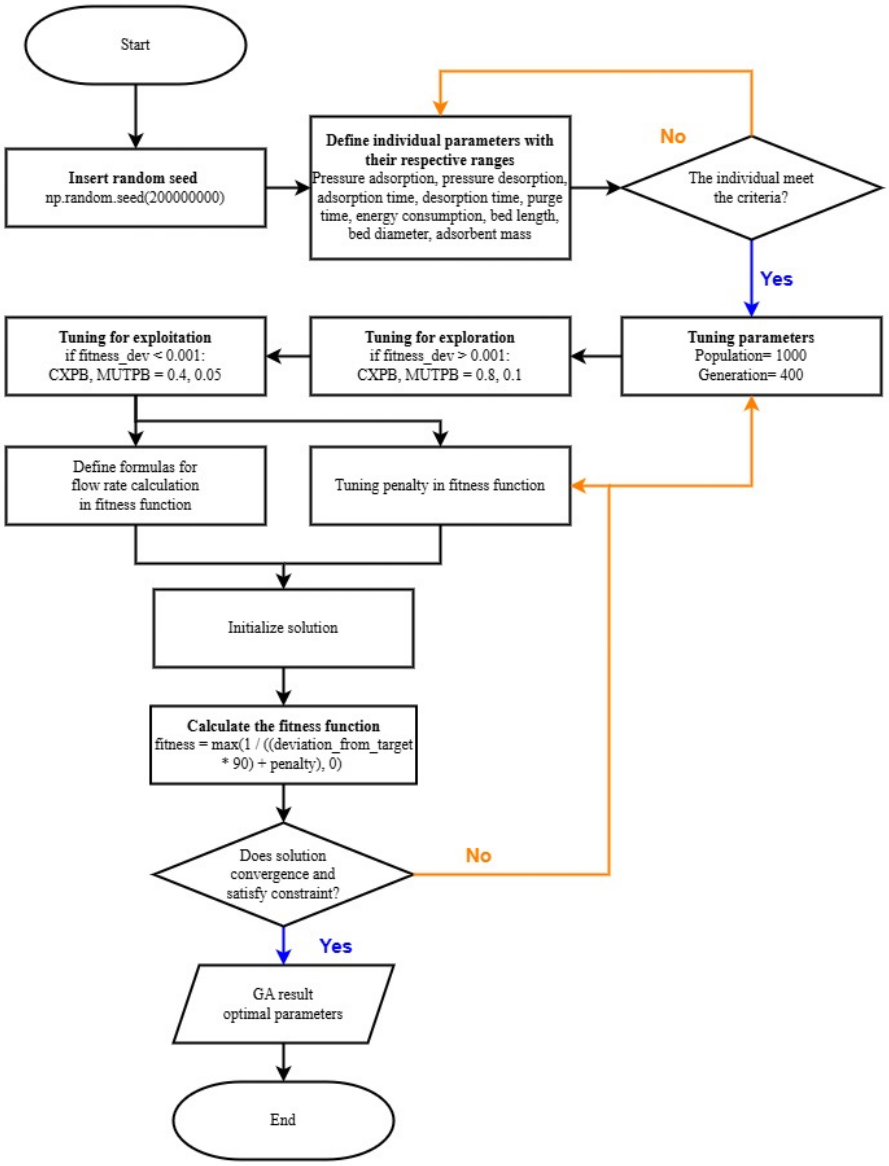

Figure 3. Genetic algorithm flowchart.

The fitness function in GA indicates the degree to which the candidate solution matches the target. The fitness value of each solution depends on how close it is to the target N_2 flow rate and how well the constraints in the algorithm are met. The penalty value is given by adding conditions that are accompanied if the resulting solution does not meet the target criteria in Table 2 and does not meet the given constraints. GA tends to try to fulfill constraints with large penalties first in finding the optimal solution. Further operations using PSO are required to validate the calculation results with GA.

2.5 Particle swarm optimization (PSO)

PSO follows the cooperative way of animal flocks (birds, fish, insects) to find food, and each member in the flock keeps changing the search pattern according to its own and other members' learning experience (Zou *et al*., 2020). The optimization process using PSO can be seen in Figure 4. In PSO, the swarm of birds is interpreted as a swarm of particles and each particle represents a candidate solution. 400 iterations were run with each iteration consisting of 1000 particles to provide enough opportunity for PSO to find the optimal solutions. A sufficient number of iterations helps achieve a convergent solution while shortening the computation time. In this study, an inertia weight of 0.6 is used to maintain a balance between exploration and exploitation during optimization. This value was chosen because it is enough to prevent premature convergence, but not so high that it still allows the search for more optimal solutions. Particles are manipulated based on Eq. (9) dan Eq. (10).

$$V_{id} = w.V_{id} + c_1.rand(\,).\,(p_{id}\text{-}x_{id}) + c_2.Rand(\,).\,(p_{gd}\text{-}x_{id}) \quad (9)$$

$$S_{id} \approx S_{id} + v_{id} \quad (10)$$

where, c_1 is the individual learning coefficient, c_2 is the social learning coefficient, rand () and Rand () are two random functions in the range [0,1] and w is the inertia weight. In this study, the value of c_1 used is 1.5 and c_2 is 2. The selection of this value aims to make PSO tend to explore the solution space globally first before exploiting.

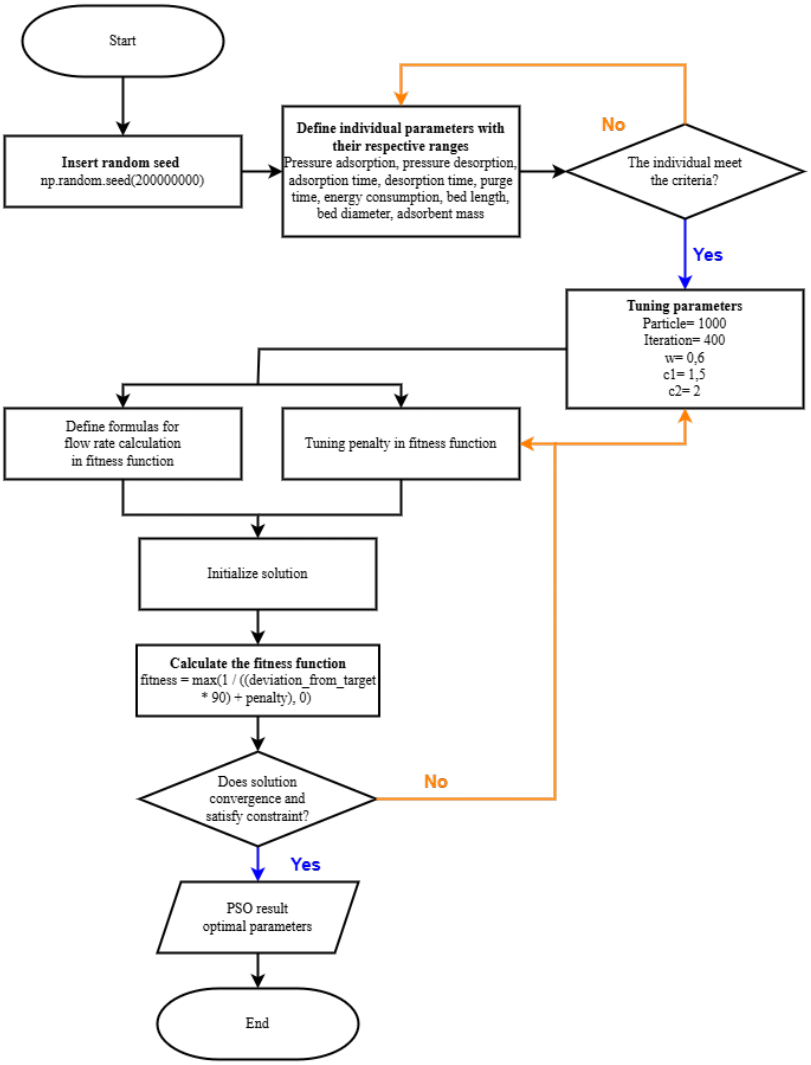

Figure 4. Particle swarm optimization flowchart.

2.6 NPT monte carlo (NPT-MC) validation

The NPT-MC simulations were carried out to simulate the adsorption of oxygen molecules within the porous material at temperatures and pressure according to literature and MHA results. Adsorption simulation on zeolite 13X framework were performed by NPT ensemble provided by the software RASPA2 (Cao *et al*., 2021). NPT-MC involves models for both adsorbent and adsorbate, using force fields to describe the energetic interactions between the molecules. The interactions of each molecule and adsorbent have been determined by calculating using the Lennard-Jones (LJ) interaction potential energy. The LJ parameters ε and σ used in the simulations are in Table 4. Potentials such as translation and reinsertion were considered for each molecule. Lorentz-Berthelot mixing rules were used to determine the strength and size parameters that describe the potential as follow:

$$\varepsilon_{xy} = \sqrt{\varepsilon_x \varepsilon_y} \quad (11)$$

$$\sigma_{xy} = \frac{1}{2}(\sigma_x + \sigma_y) \quad (12)$$

where ε_{xy} is the depth of potential energy and σ_{xy} is the collision diameter (Å) of atom or molecule x and y.

The FAU_SI framework is the most suitable for representing zeolite 13X in NPT-MC simulation. This framework defines the faujasite silica crystal structure of zeolite 13X and contains Al and Na^+ which determine the adsorption properties and surface characteristics. The helium void fraction uses a value of 0.4 according to the porosity of adsorbent, indicating the fraction of available void space within the framework that can be accessed by the O_2 during adsorption.

Table 4. Lennard-Jones potential function parameters

Molecule	Site	ε (K)	σ (Å)
Zeolite 13X framework	O	78.00	2.890
	Si	64.41	4.009
	Al	65.42	4.390
Zeolite Cations	Na^+	805.66	1.900
O_2	O	43.28	3.106
N_2	N	34.72	3.321
Ar	Ar	124.07	3.380

Each simulation of different pressure conducted of 30000 cycles. The simulation was conducted using a 1×1×1 unit cell, ensuring a representative structure for the adsorption process while maintaining computational efficiency. During simulations, the equilibrium was supposed to be obtained while the relative errors between the adsorption amounts from MHA result and NPT-MC simulations are <5%. In order to improve the visualization of the NPT-MC simulation results, iRASPA2 software was used, which provides structural visualization capabilities for the analysis of the obtained structural information and to confirm that O_2 does indeed enter the pores of the adsorbent as shown in Figure 5.

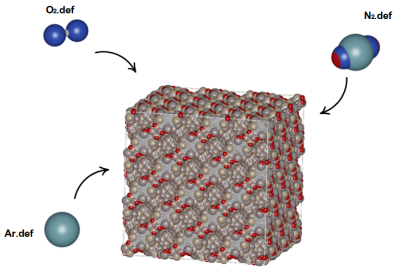

Figure 5. iRASPA2 visualization of NPT-monte carlo result.

2.7 Sensitivity analysis of process parameters

Determining the sensitivity value of each variable in the separation process is effective by involving Artificial Neural Network (ANN) modeling. Garson weight interpretation is used in understanding how strongly the influence of input variables in ANN contributes to the output. Garson's algorithm computes the relative importance of each input network based on absolute weight values which can be seen in Eq. (13).

$$Garson_{ik} = \frac{\sum_{j=1}^{h} \frac{|w_{ij}||v_{jk}|}{\sum_{i=1}^{n}|w_{ij}|}}{\sum_{i=1}^{n}\sum_{j=1}^{h} \frac{|w_{ij}||v_{jk}|}{\sum_{i=1}^{n}|w_{ij}|}} \quad (13)$$

where, $Garson_{ik}$ represent the relative importance of the *i*th input variable concerning the *k*th output neuron, w_{ij} is the connection weight between the *i*th input variable and the *j*th hidden neuron; v_{jk} representes the connection weight between the *j*th hidden neuron and the *k*th output neuron.

Before initiating the Garson weight, the GA-PSO optimization result data is adjusted to the appropriate scale by normalization to avoid the dominance of variable with bigger scale on the ANN model. Next, the ANN model was trained and divided into input_columns = ["adsorption pressure", "desorption pressure", "adsorption time", "desorption time", "purge time", "bed length", "bed diameter", "adsorbent mass"] and output_columns = ["purity", "flow rate", "energy consumption"]. The ANN model used Multi-Layer Perceptron (MLP) regressor where the weights between layers are calculated after the model reaches convergence. The weights of the ANN training results are taken from the input connection to the hidden layer (w_{ij}) and from the hidden layer to the output layer (v_{jk}). The absolute values of these two weights are then multiplied and summed for each hidden neuron to obtain the relative importance of each input variable to the output. The results of the Garson weight sensitivity calculation are then normalized by summing up all the contributions of the input variables and dividing them by the total influence, thus obtaining the results of the sensitivity value in the form of percent (%) which can be compared between process variables.

3. Result and Discussion

3.1 Effect of pressure on performance

Higher Pads increases the driving force for O_2 uptake, leading to a higher N_2 purity in the product stream because less oxygen breaks through the bed. Furthermore, the selectivity of zeolite 13X for O_2 over other gases was found to be higher at higher pressure. It can be seen from Figure 6a that PSO optimization results showed the best value for adsorption pressure at 12.752 bar, while GA gave the best adsorption pressure value at 12.827 bar. From the above results, it can be concluded that both heuristic methods produce an optimal range of adsorption pressure values in terms of adsorption capacity and energy. This shows that adsorption pressure outside this temperature range does not provide proportional benefits for the target criteria (Bulfin *et al.,* 2021). Pressure above this range does not significantly increase the adsorption capacity, but instead wastes energy that could have been minimized.

Lower pressure leads into the release of adsorbed O_2 gas from the adsorbent pores to be discharged out of the system. Figure 6b shows the PSO optimization results that obtained the best desorption pressure at 0.786 bar, while the GA results obtained at a pressure of 0.854 bar. The error in the desorption pressure variable obtained is 7.998%, this error value is greater than the adsorption pressure result. This shows that desorption pressure is more sensitive to small changes because it is influenced by several complex factors such as desorption kinetics and gas diffusion. In addition, pressures in this range are considered capable of providing optimal adsorbent regeneration capabilities so that adsorbent performance is maintained every cycle. Good regeneration leads into achieving the target amount and purity level of N_2 product (Spatolisano & Pellegrini, 2023).

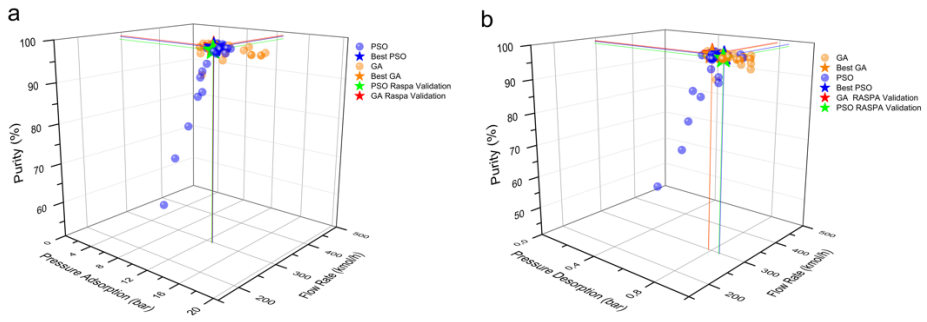

Figure 6. Comparison of GA and PSO optimization results for (a) adsorption pressure and (b) desorption pressure. Higher adsorption pressures enhance O_2 uptake and N_2 purity, while lower desorption pressures improve regeneration efficiency and reduce energy consumption.

The efficiency of pressure rise and fall is considered in achieving efficient adsorption and desorption steps. Efforts in increasing and decreasing pressure require energy consumption depending on the distance between P_{ads} and P_{des}. The scatter plot energy consumption for the PSA system can be seen at Figure 7. In the MHA results, it can be seen that GA and PSO show the same trend where the greater the pressure during the adsorption stage is followed by an increase in the energy used for compression. However, at the desorption stage, as the P_{des} gets closer to atmospheric pressure (1 bar), the energy consumption is lower. This is because the vacuum pump system will work harder to lower the pressure after the adsorption stage (Chen & Ahn, 2021). Cycles with a larger pressure difference (ΔP) are inefficient in terms of energy consumption, making them unsuitable for building a sustainable nitrogen production system to supply the small-scale ammonia industry. Kinetically, optimized desorption and adsorption pressures minimize mass-transfer resistance, maintaining favorable cycle times and increasing the overall productivity of the PSA process. These results highlight the synergy between adsorption thermodynamics, cycle kinetics, and the meta-heuristic optimization outcomes in achieving energy-efficient nitrogen production (Benkirane *et al.*, 2024). Thermodynamically, this improvement can be attributed to the enhanced adsorption potential at higher Pads and the reduced irreversible work losses during pressure reduction

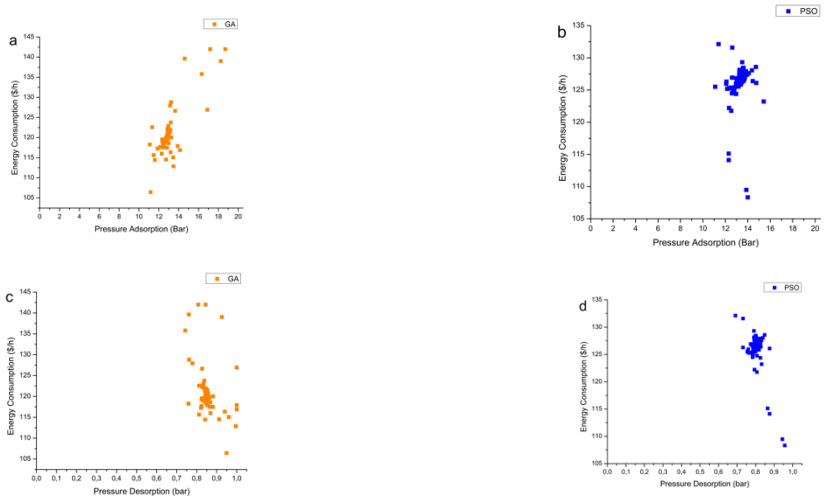

Figure 7. Scatter plots GA- PSO result (a) Energy consumption vs. adsorption pressure for GA, (b) Energy consumption vs. adsorption pressure for PSO, (c) Energy consumption vs. desorption pressure for GA, and (d) Energy consumption vs. desorption pressure for PSO.

3.2 Influence of cycle time

Cycles that are too short tend to increase the frequency of pressure rise and fall that leads to higher energy consumption. However, the cycle time, especially in the adsorption stage, is too short, causing

the O_2 content to not have enough time to be completely absorbed by the adsorbent (Benkirane *et al.,* 2024). The incomplete absorption process reduces the purity of N_2 due to the presence of other unwanted molecules. The optimization trend in Figure 8a shows that both GA and PSO consistently favor relatively long adsorption steps (727–779 s). This time range provides mass-transfer completion, which reduces early O_2 breakthrough and directly improves N_2 purity. Similarly, in the Figure 8b the desorption period (205–218 s) selected by both algorithms indicates that regeneration is the most critical stage controlling the working capacity of the adsorbent. Adequate t_{des} allows the adsorbed O_2 to fully desorb, restoring the pore volume and increasing working capacity in the next cycle. This explains why insufficient desorption time leads to incomplete regeneration, increased mass-transfer resistance, and higher energy consumption in subsequent compression steps. As a result, a lot of adsorbates is still left behind and directly affects the adsorption capacity of the next cycle. In contrast, excessive long desorption adds no significant benefit but increases energy use due to extended vacuum operation (Aly *et al.,* 2025). The optimized purge duration of (82–87 s) demonstrates that only a moderate purge time is necessary to remove remaining O_2 and Ar after desorption. Adequate purge ensures adsorbent cleanliness, preventing impurity accumulation across cycles (Bulfin *et al.,* 2021). However, longer purge times would waste product N_2 and lower recovery. MHA results on cycle time show sufficient time to perform effective separation, but not too long so as not to reduce N_2 production per unit time and purity.

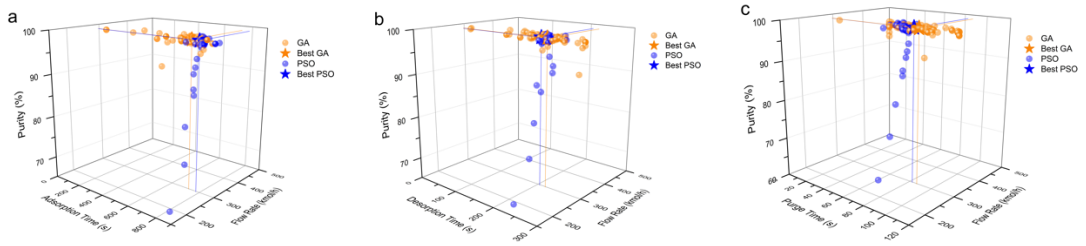

Figure 8. Distributions of GA and PSO optimization result for (a) adsorption time, (b) desorption time and (c) purge time.

3.3 Effect of volume bed

The volume size of the adsorbent bed affects the amount of O_2 adsorbed. Figure 9a shows the optimal bed length of 1.777 m from PSO and 1.906 m from GA. A small bed is in line with the objective of the small-scale NH_3 industry, but there is a decrease in efficiency. This is due to axial dispersion, which means the gas velocity must decrease on shorter beds to keep the same residence time. The Peclet number changes from linear to quadratic as the velocity decreases because the system switches from the dominance of turbulent mixing to molecular diffusion (Aly *et al.,* 2025). As a result, the effect of axial dispersion is greater than convection, resulting in a decrease in PSA performance. Meanwhile, if the bed length is too short, it will reduce the capacity of the adsorbent that can be used in the system. As a result, the adsorption rate is not maximized and the adsorbate will contaminate the N_2 product. Meanwhile, as illustrated in Figure 9b, the calculation results through GA and PSO showed the optimal range values for bed diameter at 0.582 m and 0.613 m. Bed diameter is directly related to the velocity of gas flowing in the bed. Too small a diameter can increase feedgas velocity but decrease adsorption efficiency. The gas can pass through the adsorbent too quickly, causing early O_2 breakthrough and decreased purity. These findings are consistent with the results of (Bulfin *et al.,* 2021) who reported that PSA performance declines when column diameter is not optimized to control superficial velocity and maintain uniform flow distribution. Judging from the optimal results above, the L_{bed}:d_{bed} ratio of 3:1 shows the typical characteristic of well-designed PSA units, particularly for zeolite-based air separation systems. Ratios in this range have been reported in multiple studies as optimal for balancing axial dispersion, pressure drop, and bed utilization efficiency (Akulinin *et al.,* 2020).

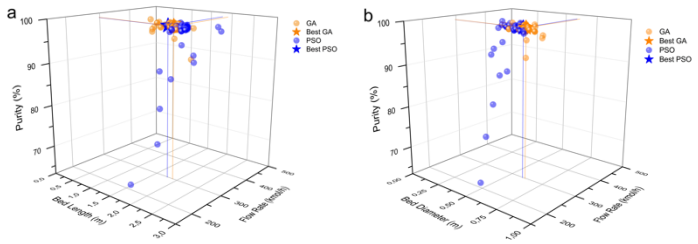

Figure 9. Distributions of GA and PSO optimization result for (a) bed length and (b) bed diameter.

3.4 Effect of adsorbent mass

Adsorbent mass is directly correlated with the adsorption capacity of the system. Figure 10 shows the GA and PSO result (76.36–84.36 kg) falls within a typical range required to maintain a stable mass-transfer zone in zeolite-based PSA air separation systems. This amount of adsorbent provides sufficient working capacity to delay the breakthrough front and ensures that O_2 and Ar are fully captured before reaching the product end of the column. Prior studies have shown that increasing adsorbent inventory enhances adsorption capacity but exhibits diminishing returns once the bed geometry and operating pressures are fixed, since additional mass no longer contributes significantly to further breakthrough delay (Benkirane *et al.,* 2024). This trend is consistent with the small error observed between the GA and PSO results (9.485%), confirming that the adsorbent mass is a less sensitive parameter than other parameters, provided that the adsorbent layer dimensions are well designed. The charge density of Zeolite 13X adsorbent, where balancing working capacity, pressure drop, and regeneration efficiency is the primary goal, is also consistent with the optimized mass range. While too much adsorbent mass will shorten breakthrough time and compromise N_2 purity, too much mass will increase pressure drop and decrease cleaning efficiency (Bulfin *et al.,* 2021). The chosen mass range is an effective configuration that maintains high separation performance without resulting in needless energy penalties or pressure drops, according to the agreement between GA and PSO outputs.

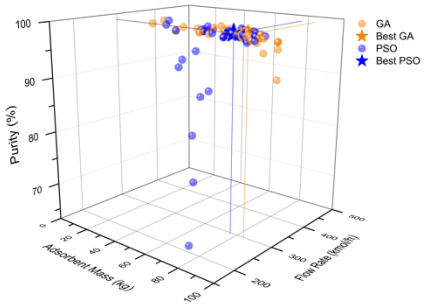

Figure 10. Distributions of GA and PSO optimization result for adsorbent mass

3.5 Fitness analysis

The fitness value results of GA and PSO show that the two heuristic methods use different approaches. Where, GA explores a wider solution space that requires a long convergence time. Based on the graph in Figure 11a and Figure 11b GA starts exploiting at >200th generation. In contrast to PSO, the algorithm experiences exploitation earlier at iteration 110. Exploitation and swarm flight speed are more prioritized in finding the best solution. Despite using different approaches, the optimal results produced by the two algorithms have an error of <10%. With an error of less than 10%, the optimization results obtained from both algorithms can be categorized as a near-optimal solution for the PSA system. This value indicates that the resulting parameters have achieved a balance between nitrogen separation efficiency and energy consumption, in accordance with the predefined optimization constraints and objectives. Therefore, the summary of optimal parameter from MHA result can be seen in Table 6, this information can be serve as a basis for guiding the design and operation of PSA for the production of high-quality N_2.

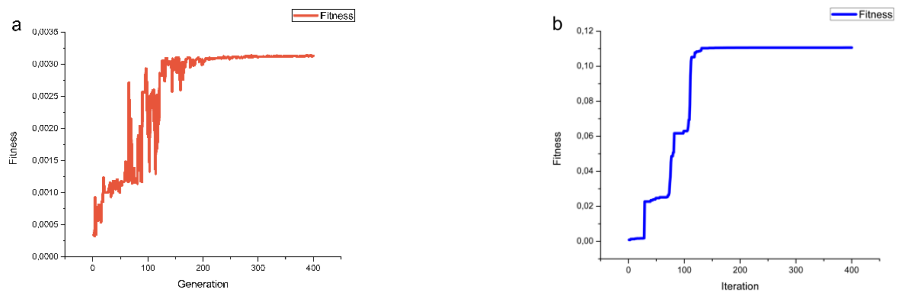

Figure 11. Comparison of fitness value (a) GA and (b) PSO.

Table 6. Optimal GA-PSO parameter result for small-scale PSA

Parameters	PSO	GA	Error (%)
Adsorption pressure (bar)	12.752	12.827	0.585
Desorption pressure (bar)	0.786	0.854	7.998
Adsorption time (s)	779.107	727.832	7.045
Desorption time (s)	205.003	218.865	6.334
Purge time (s)	82.656	87.007	5.001
Bed length (m)	1.777	1.906	6.783
Bed diameter (m)	0.582	0.613	5.057
Adsorbent mass (kg)	76.359	84.360	9.485
Target			
Energy consumption ($/h)	125.217	119.867	4.463
Purity (%)	98.944	98.980	0.036
N_2 product flow rate (kmol/h)	298.100	297.999	0.034

3.6 Validation result

NPT-MC simulations were run using the MHA pressure results in PSO and GA. Simulation results with input pressure 12.752 bar (PSO result) obtained an adsorption capacity value of 2.769 mol/kg, while using a pressure of 12.827 bar (GA) result of 2.85 mol/kg. Comparison of MHA and NPT-MC results can be seen in Figure 14. From the above comparison, the amount of O_2 adsorption, N_2 product flow rate and purity produced has an error of <3% and the level of uncertainty in adsorption capacity from five independent simulation runs, showing a deviation below ±2.5%. This alignment confirms that the optimal pressures derived from the meta-heuristic model correspond to realistic adsorption behavior on zeolite 13X. The minimal variation in adsorption capacity across methods further demonstrates that the PSA operates within the appropriate thermodynamic range for effective O_2 uptake. Overall, the NPT-MC results provide a robust validation of the MHA outcomes, confirming that the optimized PSA parameters remain reliable when evaluated at the molecular scale.

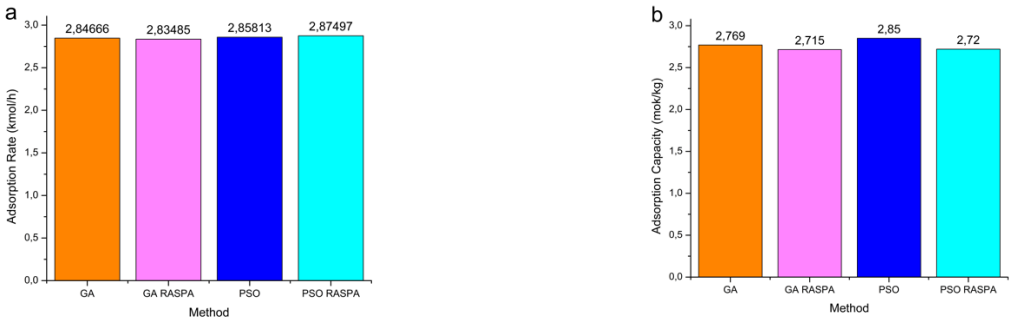

Figure 12. Validation results from RASPA2 simulation.

3.7 Comparison with other published parameter result

A comparison of the results of the parameter configuration from the baseline with the MHA GA-PSO results can be seen Figure 13. The optimization of PSA parameters has led to a significant

improvement in nitrogen (N_2) flow rate. Before optimization, studies by Benkirane *et al.* (2024), Aly *et al.* (2025), and Bulfin *et al.* (2021). demonstrated moderate N_2 flow rates, ranging from approximately 44.3 to 131.3 kmol/h. Meanwhile optimization result, GA-PSO there was a remarkable increase in N_2 flow rate, reaching around 298 kmol/h. Both GA and PSO produced comparable improvements, significantly outperforming the previously published methods. This is because the optimized pressure is sufficient to significantly increase the adsorption capacity and adsorption rate of zeolite 13X.

The purity and energy consumption values in these studies varied, achieving high purity at the expense of increased energy usage. However, the results indicate that their PSA configurations were not fully optimized for maximizing N_2 production while minimizing energy consumption. GA-PSO produced comparable improvements, significantly outperforming the previously reported methods. Additionally, the energy consumption in the optimized cases was maintained at a relatively moderate level demonstrating the efficiency of these heuristic optimization techniques. Purity values also remained stable or improved, suggesting that optimization did not compromise product quality. This highlights the effectiveness of GA and PSO in enhancing PSA performance for nitrogen separation. By adjusting key process parameters, GA and PSO successfully maximized nitrogen flow while maintaining N_2 purity level and keeping energy consumption within acceptable limits. The findings align with prior studies advocating for advanced optimization approaches in PSA-based nitrogen production. Future work may focus on refining these optimization algorithms to further enhance performance and explore real-world applications of the optimized PSA configurations.

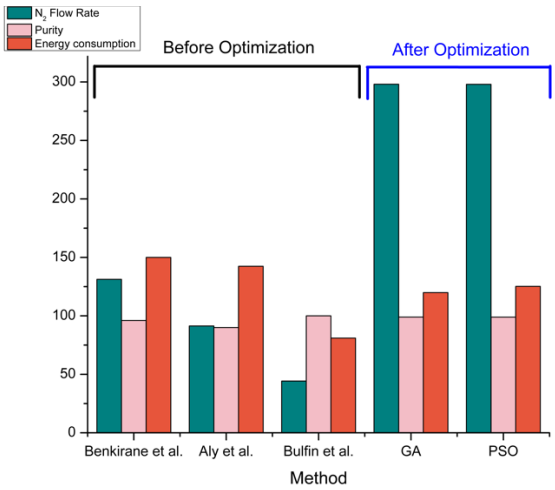

Figure 13. Comparison of N_2 flow rate, purity, and energy consumption from different PSA parameters before and after optimization.

3.8 Influence of process variables on target criteria

The analysis of the influence of process variables on target criteria, as presented in Table 7, reveals significant insights into the sensitivity levels of various parameters in the adsorption process. The sensitivity analysis result reveals that bed length has the highest influence on the 3 target criteria. Therefore, small changes in bed length design could lead to significant impact on PSA process. To maximize the purity of N_2 obtained from the separation process, this variable needs special attention. A well-proportioned design prevents excessive turbulence in the flow which reduces the contact time of the feed gas with the adsorbent, thus increasing purity. In addition, a large bed length allows for the treatment of more feed gas thereby increasing production per unit time. However, longer and wider beds tend to require more power for gas pumping from the compressor and vacuum to reach a certain pressure.

Desorption time here has a higher sensivity value than other stages because it is related to adsorbent regeneration. Meanwhile, other cycles such as purge time have the least sensitivity value because, the adsorption process tends to reach equilibrium relatively quickly, so changes in adsorption time do not have a significant impact on purity, product flow rate, or energy consumption.

Higher pressure increases the adsorption ability of zeolite but also increases the load on the compressor, so it needs to be optimized to balance performance and energy efficiency. Adsorbent mass does not have as dominant an influence as other variables and tends to have the same influence on the 3 target criteria, this is because the role of adsorbent mass as an absorbent medium depends on the influence of operating pressure, time and design in separating N_2. So that when sorted from the most sensitive variables (average) to the targets that are a priority of attention in the implementation of this technology in the future, such as, [$l_{bed} > t_{des} > P_{des} > m_{adsorbent} > P_{ads} > d_{bed} > t_{purge} > t_{ads}$]. To ensure the reliability of the ANN–Garson sensitivity model, performance metrics were evaluated. The trained ANN model achieved an R^2 value of 0.983 for purity, 0.978 for N_2 product flow rate, and 0.975 for energy consumption prediction. The corresponding RMSE values were 0.016, 0.022, and 0.019, respectively, indicating strong agreement between predicted and actual outputs. These metrics confirm that the ANN model provides a robust representation of the PSA system behavior and that the Garson weight interpretation accurately captures variable influence patterns.

Table 7. Sensitivity analysis results of operational parameters on target performance criteria.

Variable	Sensitivity level to target criteria (%)		
	Purity	N_2 product flow rate	Energy consumption
Adsorption pressure	12.94	13.13	12.54
Desorption pressure	12.79	12.80	13.87
Adsorption time	6.95	6.76	7.89
Desorption time	13.53	13.43	12.84
Purge time	10.02	10.07	9.63
Bed length	18.14	18.61	17.02
Bed diameter	12.66	12.23	13.30
Adsorbent mass	12.97	12.98	12.92

3.9 Implication MHA and future challanges

Comprehensive optimization results underscore how MHA reshape the PSA behavior of small-scale nitrogen production. It is not just about finding optimal values, but rather, through the GA-PSO framework, some distinct patterns of interaction among pressure levels, cycle durations, and adsorbent mass start surfacing that are not possible in traditional trial-and-error or single-objective tuning. The convergence of both algorithms toward similar operating windows implies the presence of a hidden optimal regime where adsorption-desorption equilibria, working capacity, and energy demand get strongly interlinked. This nonlinearity is consistent with the insights reported by Bulfin *et al.* (2021) and Benkirane *et al.* (2024), in particular those related to the sensitivity of pressure and the dominating influence of bed geometry on productivity. The model also reveals several hitherto rarely discussed system behaviors, such as enhanced long-term capacity retention with desorption pressure and disproportionate energy penalty with small deviations in adsorption pressure. These provide leads for further investigation: adaptive cycle scheduling, real-time optimization via reinforcement learning, and hybrid PSA configuration using renewable-powered compressors. Needless to say, key challenges persist-adsorbent aging, transient load variation, and control stability-but these provide a starting point for evolving much-needed resilience and intelligence in PSA systems tailored for decentralized green ammonia production.

4. Conclusion

This study developed a meta-heuristic framework, based on GA-PSO, to optimize nitrogen production in a small-scale PSA system for decentralized green ammonia. The optimized parameters allow for the target N_2 flow rate (297.999–298.100 kmol/h), high purity (98.944-98.980%), and

moderate consumption of energy (119.867-125.217 $/h). The results derived from both GA and PSO are in close alignment, with errors less than 10%, ensuring stable convergence and reliable optimization performance. Detailed sensitivity analysis has revealed that the bed length, desorption time, and pressure conditions are the major influential variables for purity and productivity as well as energy use. In addition, validation using NPT-MC confirmed that the optimized pressures fall within the <3% deviation of adsorption behavior on zeolite 13X. In general, the findings prove that meta-heuristic optimization promotes better PSA efficiency and identifies PSA feasibility in small-scale green ammonia applications. Future research could explore hybrid optimization approaches combining GA and PSO to leverage the strengths of both methods. Additionally, experimental validation of the optimized PSA parameters would further strengthen the applicability of the findings to industrial-scale operations. .

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