ARTICLE

Simulation and Optimization of Urban Small-Scale Centralized Bio-Gas Purification Process Based on Methyl Diethanolamine Absorbent

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ABSTRACT: This study addresses the energy-intensive challenge of small-scale biogas upgrading by optimizing a chemical absorption process employing methyl diethanolamine (MDEA). Focusing on a typical distributed application of 300 Nm^3/d, we developed an integrated simulation-optimization framework using Aspen HYSYS 14.0 to systematically evaluate the effects of critical operating parameters—absorption pressure, MDEA concentration, flow rate, temperature, number of trays, and reboiler duty—on methane purity and energy consumption. The key finding is the identification of an optimal parameter set: absorption pressure of 1200 kPa, MDEA concentration of 20 mol%, lean flow rate of 2.5 kmol/h, temperature of 298.15 K, 20 absorber trays, 10 regenerator trays, and a reboiler duty of 4 kW, which enabled the product gas to achieve a high CH$_4$ concentration of 97 mol%, compliant with pipeline standards. A detailed energy consumption analysis revealed that the reboiler is the most energy-intensive unit, accounting for 75.40% of the total 5.29 kW energy consumption, followed by the gas compressor (23.38%). The specific energy consumption for CH$_4$ recovery and the Energy Consumption Index (ECI) were quantified at 0.8852 kWh/kg CH$_4$ and 6.82, respectively. This work provides a validated optimization strategy and critical energy breakdown, offering practical guidance for enhancing the technical and economic viability of small-scale, centralized biogas purification systems.

KEYWORDS: Chemical absorption process; CO$_2$ capture; bio-gas; optimization; MDEA

1 Introduction

Biogas is a renewable energy source that offers an alternative solution to the world's ever-growing energy demands, while also aiding in waste reduction and greenhouse gas (GHG) emissions [1]. It is considered carbon-neutral because the carbon in biogas originates from organic materials (feedstocks) that capture carbon from atmospheric CO$_2$ over a relatively short period [2]. In addition to CH$_4$, biogas typically contains 25–45 mol% CO$_2$ and trace amounts of volatile organic compounds [3–5]. CO$_2$ is a persistent gas that reduces the density and calorific value of biogas [6]. To enhance the calorific value of raw biogas and improve its quality for more complex end uses, it is often necessary to reduce its CO$_2$ content before utilization [7,8]. Currently reported biogas purification technologies include chemical absorption [9], pressure swing adsorption [10], cryogenic separation [11], membrane separation [1], and hydrate-based separation [12]. Compared to other technologies, chemical absorption offers advantages such as high absorption capacity per unit volume of absorbent and high gas purification efficiency, making it

the leading biogas purification technology. However, it is also characterized by high energy consumption for heating the rich absorbent during regeneration [13]. When using amines for chemical absorption, the chemical reactions exhibit strong selectivity, resulting in methane (CH_4) losses below 0.1% and achieving methane concentration of 99% [14,15]. Typical operating parameters include a temperature of 120°C and a pressure of 1–2 bar [16]. However, due to evaporation necessary in the process, some amine solution is lost and requires replacement [17]. Separating CO_2 from the regenerated solution is achieved through steam heating, which returns CO_2 to the gas phase, involving significant energy consumption [18]. Some authors have achieved nearly 30% reduction in energy consumption while achieving 90% CO_2 capture efficiency [19]. The typical loading capacity of most amines is approximately 0.5–1.0 moles of CO_2 per mole of amine [20]. In terms of consumption, water, electricity, and various compounds are required. Electricity consumption depends on the operational capacity of the unit, with minimum electricity consumption at maximum load approximately 0.12 $kWh/Nm^3/h$, and maximum electricity consumption at minimum load approximately 0.14 $kWh/Nm^3/h$. Furthermore, the desorption tower requires heat for amine regeneration, consuming approximately 0.55 $kWh/Nm^3/h$ of biogas [21]. The advantages of the chemical absorption process stem from CO_2's high selectivity towards amines, resulting in significantly reduced volume of absorbent solution. For instance, chemical absorption can dissolve CO_2 in the range of 1 to 2 orders of magnitude per unit volume. On the other hand, overall energy consumption can be lower if any waste heat is available for the absorption stage compared to other scenarios [15].

Common alkanolamine solvents used for biogas decarbonization include monoethanolamine (MEA), diglycolamine (DGA), diethanolamine (DEA), aminoethylethanolamine (AEEA), and formulated or activated methyl diethanolamine (MDEA). Among these, MDEA has been widely recognized as an efficient and energy-saving CO_2 absorbent for both biogas upgrading and natural gas sweetening, and it has been extensively adopted as a commercial-grade amine for CO_2 capture [22]. Compared with primary and secondary amines (such as MEA and DEA), MDEA offers several significant advantages. Recent comparative studies further highlight that MDEA provides a favorable balance between absorption capacity and regeneration energy demand among common amine solvents [23]. Firstly, it features lower operational costs. According to the findings of Borhani and Wang [24], primary and cyclic amines typically exhibit high reaction enthalpy and faster reaction rates with CO_2, while tertiary amines such as MDEA demonstrate higher absorption capacity and lower regeneration energy demand. Since solvent regeneration accounts for approximately 40%–60% of the total CO_2 capture cost in chemical absorption processes [25], MDEA presents a clear advantage in terms of economic efficiency. In a comparative study by Zhu et al. [26], the CO_2 absorption performance of four solvents—MEA, DEA, MDEA, and 2-amino-2-methyl-1-propanol (AMP)—was simulated under identical conditions using Aspen Plus. The results showed that MDEA offered the lowest operating cost, with an energy consumption of approximately 3 GJ per ton of CO_2 removed. In addition, MDEA exhibits superior chemical stability. de Ávila et al. [27] conducted a comparative evaluation of the thermal and oxidative stability of MDEA, MEA, and DEA in CO_2 capture processes. Their findings indicated that MDEA performed more stably under high temperature and high CO_2 concentration conditions, showing particular resistance to both oxidative and thermal degradation when compared to MEA and DEA.

At present, in addition to extensive research on solvent selection, a significant body of work has focused on process optimization aimed at reducing energy consumption or improving CO_2 capture efficiency. For example, Deng et al. [28] employed Aspen HYSYS simulation software to investigate the factors affecting CO_2 removal from natural gas using amine-based solvents. Their study simulated the effects of variables such as the number of trays in the absorber, operating pressure, feed gas temperature, MDEA concentration, and amine formulation. The simulation results were systematically summarized and reasonably interpreted to deepen the understanding of the process behavior. In another study, Antonini et al. [29] developed a

CO_2 capture process based on MDEA using a combination of flowsheet modification and multi-objective optimization. Applied to a hydrogen production system from natural gas, the optimized process achieved a high CO_2 capture rate of 99.8% while significantly reducing overall energy consumption. However, most of the existing research has primarily focused on large-scale applications, with limited attention to small-scale adaptability. In small-scale biogas upgrading scenarios, the absence of economies of scale often results in higher unit costs, making such systems economically less attractive [30]. Therefore, it becomes essential to compensate for scale-related disadvantages through operational parameter optimization, thereby enhancing the technical and economic feasibility of small-scale biogas purification systems [31].

In this study, focusing on small-scale urban centralized biogas (300 Nm^3/d) as the simulation target, a chemical absorption process based on MDEA absorbent was utilized to investigate the impact of different process parameters on methane (CH_4) concentration in the product and energy costs. Optimal operational parameters were selected to achieve CH_4 concentration in the product gas meeting natural gas pipeline transportation standards. Detailed analysis of the overall process energy consumption was conducted, providing technical and theoretical support for the purification of small-scale centralized urban biogas in practical applications. The simulation-based optimization approach adopted here aligns with methodologies applied in recent amine-based capture studies [32].

The main contributions of this study are as follows:

(1)   Research scale and context: This work focuses on a small-scale urban biogas purification system (300 Nm^3/d), representing a typical distributed energy application, in contrast to conventional large-scale CO_2 capture studies.
(2)   Process optimization framework: An integrated optimization approach combining Aspen HYSYS simulation and Energy Consumption Index (ECI) analysis was developed to quantify the effects of key operating parameters—absorption pressure, MDEA concentration, flow rate, temperature, and reboiler duty—on methane concentration and total energy use.
(3)   Energy consumption analysis: The study quantitatively identified the energy contribution of major process units (compressor, pumps, and reboiler) and proposed practical reduction strategies, such as waste heat recovery for solvent preheating.

Overall, the research expands current MDEA-based simulation studies by introducing a small-scale application focus, a quantitative optimization framework, and energy pathway analysis relevant to distributed biogas upgrading systems.

2 Process Construction and Research Methods

2.1 Simulation Conditions

The process used Methyl Diethanol Amine (MDEA) solution as the gas absorption solvent (lean solution). According to the reaction mechanism between CO_2 and the amine solution, it is known that the reaction is reversible. Higher pressures can promote the forward absorption reaction, increasing the absorption of CO_2. The process simulation operated under the following assumptions [33]:

(1)   The mole fractions of CH_4 and CO_2 in the feed gas were 67 mol% and 33 mol%, respectively.
(2)   The initial temperature and pressure of the feed gas were 303.15 K and 110 kPa, respectively.
(3)   The feed gas flow rate was 300 Nm^3/d.
(4)   The compressor had an efficiency of 85%.
(5)   During the operation of both the absorption column and the regeneration column, a per-tray pressure drop of 0.25 kPa is assumed.
(6)   The methane concentration in the product gas was 97 mol%.

The simulation was conducted using Aspen HYSYS 14.0 [34,35] to simulate and optimize the energy consumption and performance of the designed process. The gas–liquid reaction between CO_2 and MDEA is assumed to reach thermodynamic equilibrium within each tray, which is a reasonable approximation under typical industrial operating conditions due to the fast reaction rate of CO_2 with amines. Therefore, explicit kinetic parameters were not introduced. This assumption allows for reliable prediction of process performance and energy consumption, as validated by previous studies [26,28]. The feed biogas was simplified to a binary CO_2/CH_4 mixture, as trace components are typically removed by pretreatment and their inclusion is not central to the core CO_2/CH_4 separation mechanism studied here.

2.2 Process Overview

The absorption process consists of a gas compression unit, an absorption tower unit, and a desorption tower unit. The specific simulation flow is illustrated in Fig. 1. Biogas undergoes compression (Com-1, Com-2) and cooling (E-3, E-4) before entering the absorption tower unit (T1). The product gas, after the reaction, is discharged from the top of T1, while the MDEA rich solution exits from the bottom of T1 and undergoes pressure reduction via a pressure control valve to 110 kPa. It then undergoes heat exchange with MDEA lean solution (E-1) before entering the desorption tower (T2) for regeneration of the absorbent solution. The regenerated MDEA lean solution is pumped (Pump-2), cooled (E-2), and returned to the absorption tower for further reaction. The desorbed CO_2 (Rich CO_2) is discharged from the top of T2. In this process, the amine loss in the desorption tower is relatively low; therefore, wash trays were not installed. To maintain the system amine balance, an amine makeup point was set in stream M9 to sustain absorption performance.
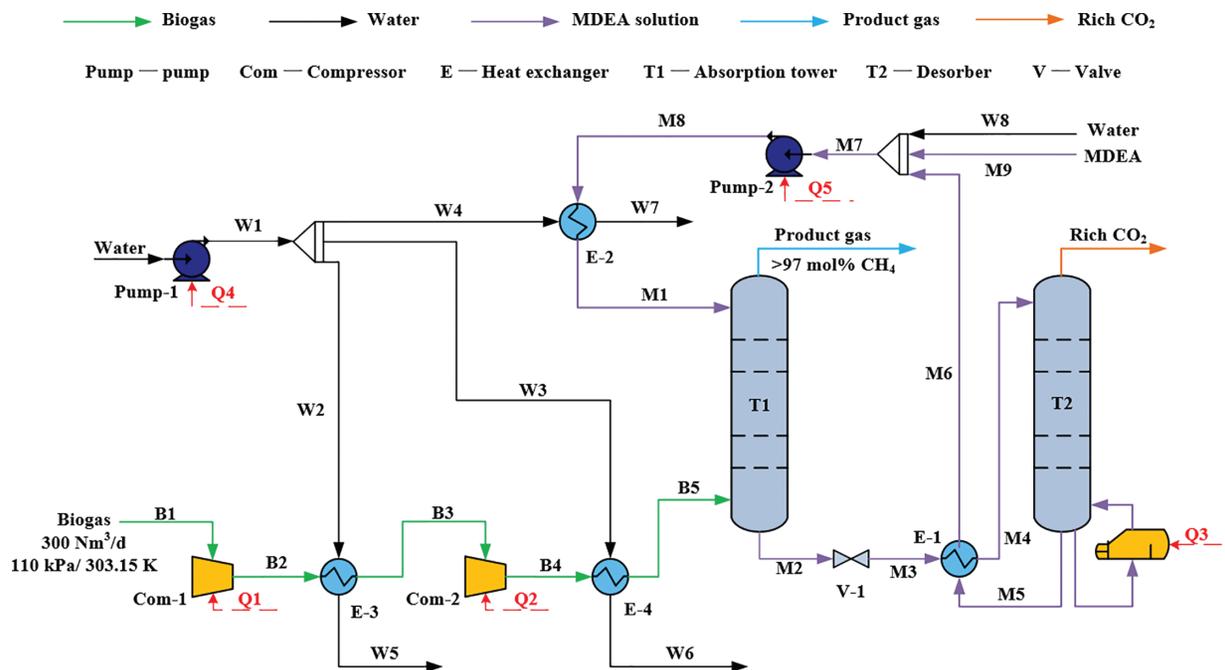

Figure 1: Process flow chart of biogas purification by absorption method

2.3 Energy Consumption Evaluation Index

2.3.1 Unit Recovery Energy Consumption

The specific energy consumption is a key performance indicator for evaluating the efficiency of gas purification processes. It is defined as the total energy consumption divided by the mass flow rate of the target gas in the product gas, as shown in Eq. (1) [33]:

$$W_{unit} = W_{total}/m_{product} \tag{1}$$

where W_{unit} is the unit CH_4 recovery energy consumption, kWh/kg CH_4; W_{total} is the total energy consumption, kW; and $m_{product}$ is the mass flow rate of CH_4 in the product gas, kg/h.

2.3.2 Minimum Separation Work

From the second law of thermodynamics, it is known that the separation of a mixture of gases is a non-spontaneous process that requires external work to meet separation requirements. Assuming the separation process is an ideal reversible process, the corresponding work requirement is minimized, known as the minimum separation work [36]. The minimum separation work represents the theoretical limit of energy consumption in the actual separation process; a higher value indicates greater difficulty in gas separation. The minimum separation work is independent of the specific separation process and primarily influenced by parameters such as the concentration of components in the feed gas, concentration of products, and recovery rate. If the feed gas contains components A and B, which are separated into products Y and Z with a recovery rate of r, the minimum separation work required can be calculated using the following formula [37]:

$$W_{min,T} = -RT \left\{ \begin{array}{c} (X_A \ln X_A + X_B \ln X_B) - r (Y_A \ln Y_A + Y_B \ln Y_B) - \\ (1-r) (Z_A \ln Z_A + Z_B \ln Z_B) \end{array} \right\} \tag{2}$$

In the equation, $W_{min,T}$ represents the minimum separation work of the system. X_A/X_B denote the concentrations of components A and B in the feed gas, respectively. Y_A/Y_B represent the concentrations of components A and B in the product gas, while Z_A/Z_B denote the concentrations of components A and B in the remaining gas phase after separation.

2.3.3 Gas Separation Energy Consumption Index (ECI)

The minimum separation work is independent of the specific separation process, but different separation process routes require varying energy consumption to achieve the same separation objectives. To evaluate the economic viability of various separation processes, the Energy Consumption Index (ECI) is used, which compares the actual energy consumption of a process to its minimum separation energy requirement. Furthermore, within the same separation process, this ratio provides insight into deviations from the ideal separation process under different separation requirements, thereby guiding the optimization of industrial process flows. The Energy Consumption Index (ECI) is obtained by dividing the actual separation work by the minimum separation work, as shown in Eq. (3) [38]:

$$ECI = \frac{W_{act}}{W_{min,T}} \tag{3}$$

where W_{act} represents the actual separation work and ECI denotes the Energy Consumption Index, which is a dimensionless quantity.

3 Results and Discussion

In the gas absorption process, factors such as operating pressure, absorbent concentration, flow rate, temperature, number of trays in the absorption tower, etc., significantly influence CO_2 absorption efficiency and the composition of the product gas. Additionally, the reboiler load in the regeneration tower affects the regeneration of the absorbent. Therefore, optimizing operational parameters of the chemical absorption unit is essential to achieve high-concentration product gas and low energy consumption.

3.1 Absorber Pressure

Higher pressure facilitated the reaction between CO_2 and the methyldiethanolamine (MDEA) solution, but it also increased compression energy consumption and equipment costs. Therefore, it was crucial to determine the appropriate absorption pressure. For simulation purposes, an MDEA absorbent concentration of 20 mol% [24,26], a volumetric flow rate of 3 kmol/h, a plate tower with 20 trays [28], and an internal pressure drop of 5 kPa within the tower were assumed [33].

The absorption process was simulated using Aspen software. Fig. 2 illustrates the effects of operating pressure in the absorption column on CO_2 absorption efficiency, methane (CH_4) concentration, and product gas yield. As the absorption pressure increases, both CO_2 absorption efficiency and CH_4 concentration in the product gas rise markedly in the medium-pressure range, while the improvement becomes progressively less significant at higher pressures. At an absorption pressure of 200 kPa, the CH_4 concentration in the product gas is 91.90 mol%, and the CO_2 absorption efficiency is approximately 88%. When the pressure is elevated to 400 kPa, the CH_4 concentration increases substantially to 96.03 mol%, accompanied by a clear enhancement in CO_2 capture capacity. However, beyond this point, the rate of improvement declines significantly. At 600 kPa, the CH_4 concentration reaches 96.81 mol%, and at 1100 kPa it increases marginally further to 97.31 mol%. Additional pressure increases yield only negligible gains in CH_4 concentration while sharply increasing compression energy consumption. This trend is consistent with the findings of Zhu et al. [26] and Deng et al. [28], who simulated natural gas decarbonization using MDEA absorbents and reported that higher pressures substantially improve CO_2 absorption efficiency and CH_4 purity. These results indicate that moderate pressures can effectively enhance CO_2 absorption due to stronger gas–liquid contact and higher mass transfer rates. However, once the system approaches equilibrium, further pressurization offers limited benefits and instead leads to higher energy consumption and capital costs. Considering the trade-off between product gas purity and energy demand, this study identifies 1200 kPa as the optimal absorption pressure for subsequent simulations. Under this condition, the CH_4 concentration in the product gas reaches 97 mol%, which meets the purity requirements for natural gas pipeline transmission.
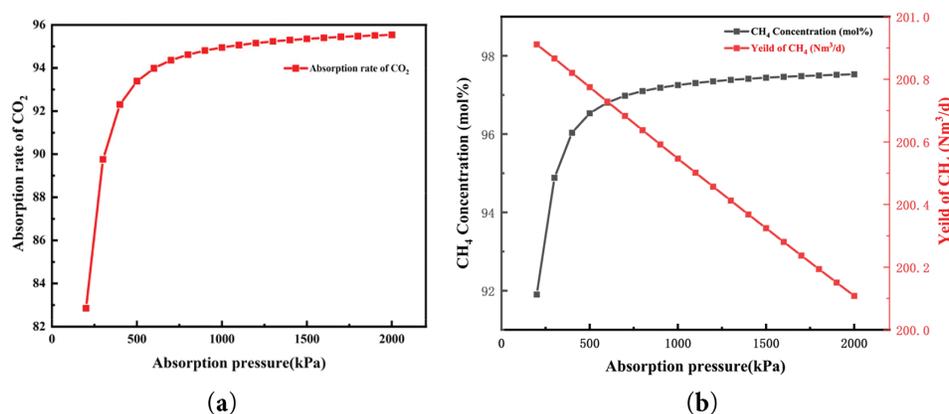

(a)   (b)

Figure 2: Influence of the pressure inside the absorber on (**a**) the CO_2 absorption rate and (**b**) the concentration and yield of CH_4

3.2 Concentration and Flow of Lean Solution

When the concentration and flow rate of the absorbent solution are constant, increasing the absorption pressure to a certain value stabilizes the CO_2 absorption efficiency. Therefore, optimization of the monoethanolamine (MDEA) absorbent solution concentration and flow rate was carried out under an absorption pressure of 1200 kPa.

After Aspen simulation calculations, the effects of flow rate on CO_2 absorption efficiency and CH_4 concentration were analyzed for lean liquid concentrations of 15%, 20%, 25%, and 30% as shown in Fig. 3. As depicted in Fig. 3, the trends of how flow rate affects CO_2 absorption efficiency and CH_4 concentration are similar across different concentrations. When the flow rate of the lean liquid is constant, increasing the MDEA concentration from 15 to 20 mol% results in increased CO_2 capture. However, further increases in the lean liquid concentration do not significantly raise CH_4 concentration; instead, there is a declining trend. This is because the higher MDEA concentration inhibits the ionization of water molecules, affecting the reactions of CO_2 and OH-, thereby reducing both CO_2 absorption efficiency and CH_4 concentration. Therefore, a lean liquid concentration of 20 mol% of MDEA is chosen for efficient CO_2 absorption. Similar non-linear effects of amine concentration on CO_2 solubility have been reported in recent thermodynamic studies [39].
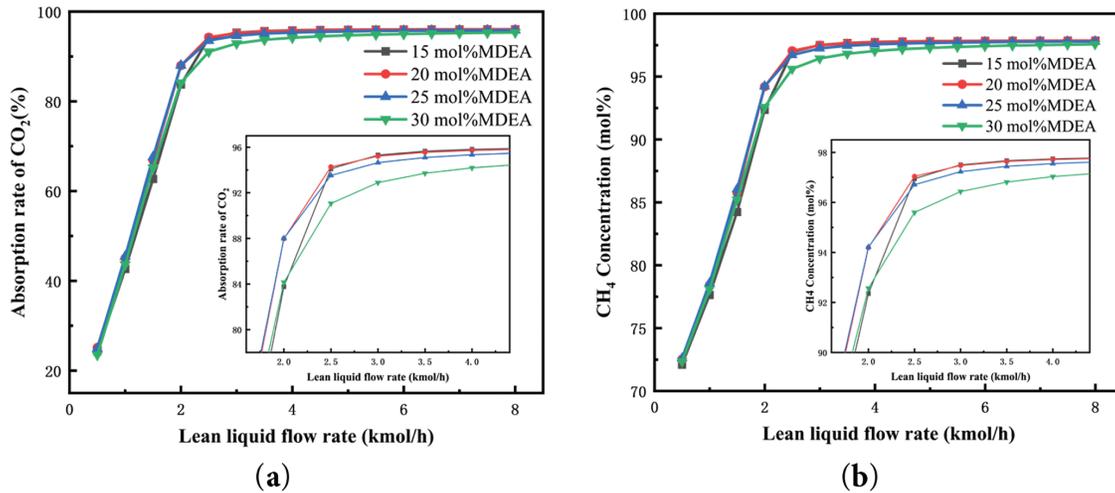

Figure 3: Influence of lean liquid concentration and flow rate on (**a**) the CO_2 absorption rate and (**b**) the CH_4 concentration in the product gas

When the lean liquid concentration is held constant, increasing the flow rate of the lean liquid results in an initial increase followed by stabilization of CO_2 absorption efficiency and CH_4 concentration. At lower flow rates of the lean liquid, the MDEA solution may not completely absorb CO_2 from the mixed gas. Increasing the flow rate of the lean liquid enhances the MDEA content, effectively promoting early-stage absorption of CO_2 by the lean liquid and rapidly increasing the CH_4 concentration. However, once the lean liquid flow rate reaches a certain threshold, mass transfer limitations restrict further reaction progress, leading to a balanced CO_2 absorption reaction. Continuously increasing the lean liquid flow rate does not significantly enhance CH_4 concentration. On the contrary, a larger amount of lean liquid increases regeneration energy consumption and circulation load, thereby raising overall operational energy consumption and CH_4 recovery energy. Under an absorption pressure of 1200 kPa, with a lean liquid of 20 mol% MDEA and a flow rate of 2.5 kmol/h, CO_2 absorption efficiency reached 94.28%, and the CH_4 concentration in the product gas was 97.04 mol%. These values meet natural gas pipeline transportation

standards. Therefore, these parameters are selected as optimal for the concentration and flow rate of the lean liquid in the absorption process.

3.3 Lean Liquid Temperature

CO_2 absorption is an exothermic reaction, and the temperature of the lean liquid entering the absorption tower affects the efficiency of CO_2 absorption and the methane (CH_4) concentration in the product gas. Therefore, this section focuses on optimizing and analyzing the temperature of the lean liquid. Based on the optimized process parameters mentioned above—absorption pressure of 1200 kPa and lean liquid concentration of 20 mol%—simulation analysis was conducted to assess the impact of different flow rates and temperatures of the lean liquid on CO_2 absorption efficiency and CH_4 concentration.

Fig. 4 illustrates the effect of the lean solvent inlet temperature on CO_2 absorption efficiency and methane concentration. As the lean solvent temperature increases, both CO_2 absorption efficiency and CH_4 concentration exhibit a similar decreasing trend, which is consistent with the findings reported by Zhang et al. [40]. In addition, the most pronounced decline is observed when the lean solvent flow rate is 2 kmol/h. CO_2 absorption by the lean liquid is an exothermic reaction, where lower temperatures favor the equilibrium shift towards CO_2 absorption. As the lean liquid temperature rises, the occurrence of reverse reactions reduces CO_2 absorption efficiency, leading to an increased CO_2 content in the product gas discharged from the top of the absorption tower and a subsequent decrease in CH_4 concentration. According to the graph, when the lean liquid flow rate is 2 kmol/h, increasing the lean liquid temperature from 303.15 to 323.15 K results in CO_2 absorption efficiency and CH_4 yield decreasing to 59.95 and 82.68 mol%, respectively. Once the lean liquid flow rate exceeds a certain value (greater than 2.5 kmol/h), increased absorption of CO_2 by more MDEA reduces the saturation of the rich liquid. Therefore, effective CO_2 absorption can still be maintained within the temperature range of 293.15 to 308.15 K. Although lower temperatures of the lean liquid can enhance CO_2 absorption efficiency and CH_4 concentration, cooling the lean liquid to low temperatures requires substantial cooling water and pump power consumption at the bottom of the regeneration tower. Additionally, in practical production, the viscosity of the solution increases with decreasing reaction temperature, leading to reduced diffusion coefficients and absorption rates. Based on the analysis above, at a lean liquid flow rate of 2.5 kmol/h, a lean liquid temperature of 298.15 K is chosen as optimal for entering the absorption tower.
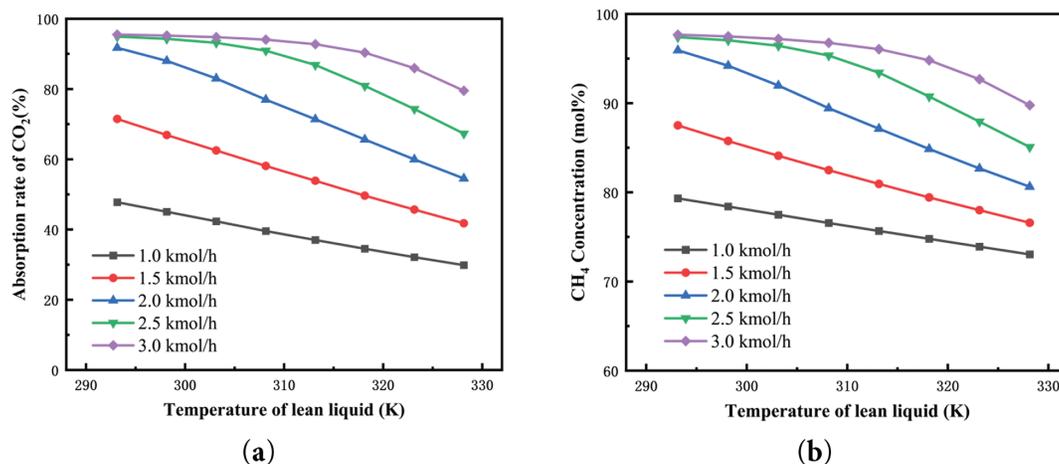

Figure 4: Influence of lean liquid temperature on (**a**) the CO_2 absorption rate and (**b**) the CH_4 concentration of product gas

3.4 Number of Absorption Trays

A tray column was selected for the absorption process, and the number of trays directly affects the mass transfer efficiency between the gas and liquid phases. Fig. 5 illustrates the relationship between the number of trays, CO_2 absorption efficiency, and methane concentration in the product gas. Under constant operating conditions—namely a lean solvent concentration of 20 mol% MDEA, temperature of 298.15 K, flow rate of 2.5 kmol/h, and absorption pressure of 1200 kPa—increasing the number of trays enhances both CO_2 absorption efficiency and CH_4 concentration. This observation is consistent with common industrial practice. The vertical axis values correspond to separation parameters at each plate level. As the number of plates in the absorption tower increases (15, 20, 25), both CO_2 absorption efficiency and CH_4 concentration show an increasing trend. Specifically, CO_2 absorption efficiencies are 88.60, 94.29, and 97.21 mol%, respectively, while CH_4 concentrations are 94.46, 97.04, and 98.43 mol%, respectively. This is because increasing the number of plates enlarges the contact area between CO_2 and the lean liquid, thereby facilitating more CO_2 absorption by the lean liquid. However, the relationship between CO_2 absorption and the number of plates is not linear. At 25 plates, CO_2 absorption by the lean liquid approaches saturation, and both CO_2 absorption efficiency and CH_4 concentration stabilize without significant increases. In addition, an excessive number of trays increases both equipment manufacturing costs and operating expenses. From an economic perspective, the number of trays is directly related to the following aspects: (1) Equipment manufacturing cost: The more trays there are, the greater the column height and the higher the complexity of the internal structure; (2) Footprint and installation cost: Increasing the number of trays leads to larger column dimensions and higher infrastructure investment; (3) Operation and maintenance cost: A greater number of trays may result in increased pressure drop (although a per-tray pressure drop of 0.25 kPa is assumed in this study), thereby raising energy consumption. Therefore, selecting 20 trays represents a reasonable techno-economic compromise, as it achieves the required CH_4 concentration in the product gas to meet the natural gas pipeline transmission standard ($\geq$97 mol%) while avoiding excessive investment and operational burden.
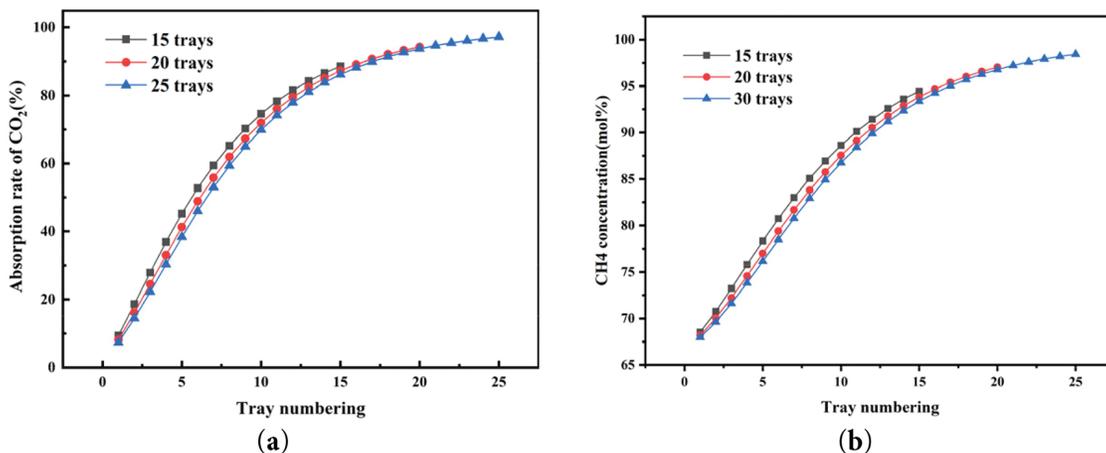

Figure 5: Influence of the number of trays on (**a**) the CO_2 absorption rate and (**b**) the CH_4 concentration of product gas

3.5 Reboiler Duty and Tray Numbers in Regeneration Tower

After the MDEA solution in the absorption tower absorbs CO_2, it undergoes heating regeneration in the regeneration tower. The regenerated MDEA lean solution is pressurized, cooled, and then returned to the

absorption tower for the next absorption cycle. The performance of the reboiler in the regeneration tower determines the regeneration capacity of the absorbent solution.

Fig. 6 depicts the effect of reboiler power on CO_2 desorption rate in the rich solution and CH_4 concentration in the product gas. As shown in the graph, increasing reboiler power initially enhances both CO_2 desorption rate and CH_4 concentration in the product gas, followed by stabilization. At a reboiler power of 3 kW, the CO_2 desorption rate reaches 89.68%, indicating that most of the CO_2 absorbed in the MDEA solution has been removed. Increasing the reboiler power to 4 kW raises the CO_2 removal rate to 99.67%. However, since the residual CO_2 in the MDEA solution is minimal at this point, further increasing reboiler power does not significantly improve CO_2 removal rate. At this stage, the CH_4 concentration in the product gas discharged from the top of the absorption tower stabilizes at 97.01 mol%, with a methane recovery rate of 99.78%. Based on the above analysis, a reboiler power of 4 kW is chosen as optimal. The choice of 10 trays in the regenerator can be justified from the following perspectives. First, unlike the absorber, the main objective of the regenerator is to fully desorb CO_2 from the rich solvent. The performance of the regenerator is relatively less sensitive to the number of trays compared to the absorber, which requires highly efficient multi-stage gas-liquid mass transfer. Therefore, increasing the number of trays in the regenerator has a limited impact on overall performance. Second, as shown in Table 1 and Fig. 6, the current configuration requires only 4 kW of reboiler duty to achieve a CO_2 removal rate of 99.67%, while maintaining a CH_4 concentration of 97 mol% in the product gas, indicating that the system is already in an efficient regeneration state. The existing 10 trays are sufficient to meet the mass transfer and separation requirements. Reducing the number of trays further would result in a CH_4 concentration in the product gas that does not meet the required standard of 97 mol%. For instance, as shown in Table 1, when the tray number is reduced to 5, the CH_4 concentration in the product gas drops to 96.9 mol%, failing to meet the 97 mol% requirement. Finally, increasing the number of trays results in higher capital costs, larger equipment size, increased reboiler duty, and pressure drop. However, the simulation results indicate that with the current 10 tray configuration, the CO_2 concentration in the MDEA rich solvent is already close to complete desorption, and adding more trays would have negligible benefits in improving the product gas purity.
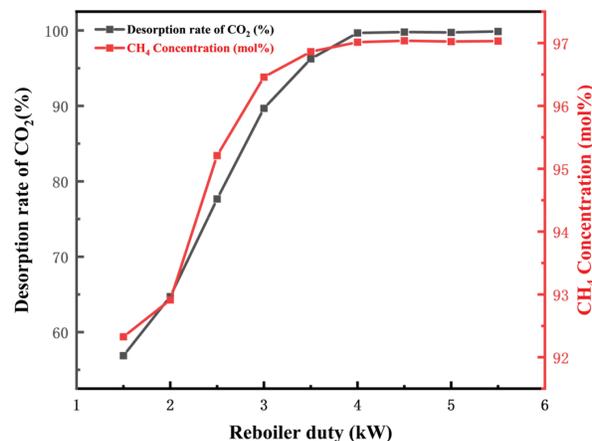

Figure 6: Effect of reboiler load on CO_2 desorption rate and CH_4 concentration of product gas

Table 2 presents the relationship between reboiler power and CO_2 desorption gas flow rate. As reboiler power gradually increases, the amount of CO_2 desorbed in the regeneration tower also increases, leading to a decrease in the CO_2 content in the product gas discharged from the absorption tower. Increasing the

reboiler load in the regeneration tower can raise the temperatures and CO_2 removal efficiency of the MDEA-rich solution before and after the heat exchanger. Therefore, enhancing the temperature of the MDEA-rich solution entering the heat exchanger can improve CO_2 removal efficiency under the same reboiler power. It should be noted that although the inlet and outlet temperatures of the lean–rich heat exchanger (E-1) vary under different reboiler duties (Table 2), the heat-exchanger configuration itself was kept constant, and the minimum temperature approach remained above 5 K. The temperature variations arise solely from process coupling rather than changes in heat-exchanger design. Therefore, optimization of heat-exchanger parameters is not included in this system-level study.

Table 1: CO_2 desorption rate and CH_4 concentration of product gas at different tray numbers of regeneration tower

Number of trays in the regenerator	CH_4 concentration (mol%)	Desorption rate of CO_2 (%)
5	96.90	98.53
10	97.01	99.78

Table 2: Relationship between reboiler duty and desorption flow

Duty (kW)	Temperature of rich liquid before heat exchange (K)	Temperature of rich liquid after heat exchange (K)	Yield of desorbed CO_2 (kmol/h)	Yield of CO_2 in Product gas (kmol/h)
1.5004	314.00	318.15	0.1540	0.02993
2.0010	316.75	321.65	0.1564	0.02764
2.5012	319.88	327.45	0.1661	0.01795
3.0024	322.13	334.85	0.1712	0.01287
3.4995	323.06	342.05	0.1729	0.01125
3.9924	323.61	345.85	0.1734	0.01064
4.4967	323.57	347.75	0.1735	0.01054
5.0069	323.59	348.45	0.1735	0.01060
5.4903	323.63	348.85	0.1734	0.01057

3.6 Energy Consumption Analysis

Based on the optimization of key absorption parameters in previous sections, the determined absorption process parameters are as follows: absorption pressure of 1200 kPa, MDEA lean liquid concentration of 20 mol%, lean liquid flow rate of 2.5 kmol/h, temperature of 298.15 K, 20 plates in the absorption tower, 10 plates in the regeneration tower, and a reboiler power of 4 kW. The initial pressure of the feed gas is 110 kPa, with a compression ratio of 10.91 before and after single-stage compression, hence employing two-stage compression with intercooling for pressurization before entering the absorption tower for reaction. Table 3 lists the optimized logistics information and Table 4 presents the parameters of the absorption process equipment units and energy consumption values, while Fig. 7 illustrates the energy consumption structure of this process. The overall energy consumption is 5.29 kW, with gas compression unit, pump transport unit, and reboiler energy consumption at 1.24, 0.667, and 3.99 kW, respectively. These correspond to 23.38%, 1.22%, and 75.40% of the total energy consumption, highlighting the reboiler and gas compression units as key energy-consuming components. The methane (CH_4) content in the product gas is 5.98 kg/h, with CH_4 recovery energy consumption at 0.8852 kWh/kg CH_4. The minimum separation work in the separation

process is 0.1297 kWh/kg CH_4, resulting in an ECI (Energy Consumption Index) value of 6.82. Increasing the temperature of the high-pressure feed gas after compression allows this heat to be utilized for preheating the MDEA-rich solution, thereby reducing reboiler power and lowering the overall energy consumption of the absorption process.

Table 3: Optimized logistics information

Stream	T/°C	P/kPa	m/(kg/h)	s/(kJ/kg·K)	h/(kJ/kg)
M1	25.00	1200.00	95.62	−7.98	−8420.01
M2	55.91	1200.00	103.25	−7.36	−8457.76
M3	50.46	110.00	103.25	−7.35	−8457.76
M4	72.70	110.00	103.25	−6.93	−8315.96
M5	107.27	110.00	94.10	−7.18	−8035.40
M6	59.74	110.00	94.10	−7.62	−8190.99
M7	60.09	110.00	95.62	−7.63	−8310.26
M8	60.26	1200.00	95.62	−7.63	−8308.84
M9	59.74	110.00	0.0021	−7.02	−3752.54
B1	30.00	110.00	14.09	−1.90	−7107.92
B2	135.01	363.33	14.09	−1.84	−6947.97
B3	25.00	363.33	14.09	−2.32	−7117.50
B4	129.74	1200.00	14.09	−2.26	−6961.25
B5	25.00	1200.00	14.09	−2.73	−7125.44
W1	20.01	200.00	735.12	−9.11	−15,881.41
Water	20.00	101.00	735.12	−9.11	−15,881.54
W2	20.01	200.00	114.46	−9.11	−15,881.41
W5	25.00	200.00	114.46	−9.04	−15,860.54
W3	20.01	200.00	110.86	−9.11	−15,881.41
W6	25.00	200.00	110.86	−9.04	−15,860.54
W4	20.01	200.00	509.80	−9.11	−15,881.41
W7	25.00	200.00	509.80	−9.04	−15,860.54
W8	59.74	110.00	1.52	−8.58	−15,715.34
Rich CO_2	79.12	105.00	9.15	−0.04	−9612.75
Product gas	25.36	1195.00	6.46	−5.83	−4989.17

Table 4: Parameters and energy consumption of main equipment

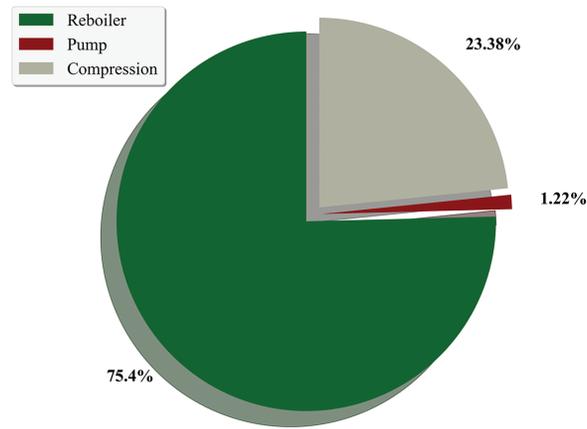| Equipment unit	Code	Medium	Flow rate (kmol/h)	Energy consumption (kW)
Compression	Com-1	Biogas	0.56	0.625
	Com-2	Biogas	0.56	0.611
Pump	Pump-1	Water	40.81	0.0278
	Pump-2	MEDA solution	2.50	0.0389
Reboiler	–	–	–	3.99
Sum	–	–	–	5.29

Figure 7: Energy consumption proportion of each unit

To further evaluate the energy consumption performance of this study, the optimized unit methane recovery energy consumption (0.8852 kWh/kg CH_4) was compared with recently published small-scale amine-based biogas upgrading systems (Table 5). It can be observed that the energy consumption achieved in this study at a scale of 300 Nm^3/d is lower than most reported MEA or mixed-amine systems, and the Energy Consumption Index (ECI = 6.82) is also at a relatively low level. This demonstrates that the MDEA solvent and parameter optimization strategy adopted in this work offer good energy consumption advantages for small- and medium-scale applications, particularly for urban distributed biogas projects sensitive to operational costs.

Table 5: Comparison of energy consumption performance for small-scale amine-based biogas upgrading systems

Reference	Time	Scale (Nm^3/d)	Solvent	ECI	Converted (kWh/kg CH_4)
[41]	2023	641	MEA	14.1	1.83
[42]	2024	720	MEA + MEG	12.2	1.58
[43]	2025	500	PZ + MDEA	11.0	1.43
This work	–	300	MDEA	6.82	0.8852

3.7 Energy Consumption Optimization Strategies

Simulation results indicate that the reboiler accounts for approximately 75.4% of the total energy consumption (see Fig. 7), making it the most energy-intensive unit in the absorption–regeneration process. In addition to the previously optimized operating parameters (e.g., number of trays, solvent flow rate, and temperature), further analysis was conducted on potential strategies such as waste heat recovery and alternative solvent formulations, as outlined below:

(1)   Feasibility and Integration Pathways of Waste Heat Recovery: In the current process, the feed gas is compressed from 110 to 1200 kPa. After two-stage compression, its temperature increases significantly (see Section 3.6). This high-temperature gas can be utilized as a low-grade heat source to partially replace the reboiler duty. Previous studies have shown that using hot compression exhaust or product gas to preheat the rich MDEA solution can substantially reduce the reboiler power demand and thereby alleviate the overall energy burden. Application recommendation: A waste-heat exchanger module can be integrated into the simulation system, where the compression exhaust is used for secondary

heat exchange with the rich solvent (e.g., by adding an auxiliary heat exchanger downstream of E-1). This would reduce the amount of external steam or electric heating required [19]. Although waste-heat recovery has strong energy-saving potential, its quantitative evaluation involves additional system modeling requirements and heat-integration design that fall outside the scope of the present study. The research will be reported in detail in future work

(2) Energy Advantages of Alternative Solvent Formulations: In the current simulation, MDEA is employed as a representative tertiary amine solvent. Although it offers high selectivity, it requires relatively high regeneration temperatures (110°C–120°C), resulting in a high reboiler load. To mitigate this issue, the following formulation strategies may be considered: Activated amine systems (aMDEA): Composite solvents formed by blending MDEA with primary amines (e.g., PZ, MEA) or polyamines (e.g., AEEA) can improve absorption rates and achieve comparable removal efficiencies with lower regeneration energy requirements [13]. Mixed-solvent systems (e.g., MDEA + TBEE): The addition of hydrophobic solvents or surfactants can reduce the specific heat capacity of the solvent and improve mass transfer characteristics, thereby significantly lowering reboiler duty while enhancing tray efficiency in the absorber [44].

Application recommendation: In follow-up simulations, part of the MDEA concentration could be replaced with aMDEA while keeping the total amine concentration constant, in order to evaluate the reduction in energy consumption. Alternatively, experimental data could be coupled with the simulation to generate regressed thermophysical parameters for mixed-solvent systems.

4 Conclusion

This study simulates a small-scale urban centralized biogas system (300 Nm^3/d) to investigate the impact of various process parameters on methane (CH_4) concentration in the product gas and energy consumption. The objective is to identify optimal process parameters for MDEA chemical absorption and provide a comprehensive analysis of energy consumption under these optimal conditions.

With an absorption pressure of 1200 kPa, a lean MDEA concentration of 20 mol%, a lean liquid flow rate of 2.5 kmol/h, a lean liquid temperature of 298.15 K, 20 trays in the absorption tower, 10 trays in the regeneration tower, and a reboiler duty of 4 kW, the methane concentration in the product gas reaches 97 mol%, meeting the natural gas pipeline transportation standards. The overall energy consumption of the process is 5.29 kW, with the energy consumption breakdown as follows: gas compression unit (23.38%), pump transport unit (1.22%), and reboiler (75.40%). The reboiler and gas compression units are identified as the primary energy-consuming components. The energy consumption per unit of methane recovered is 0.8852 kWh/kg CH_4, with an Energy Consumption Index (ECI) of 6.82.

This study specifically addresses small-scale urban centralized biogas systems (300 Nm^3/d), which are being progressively deployed in urban-rural transition zones in China. These systems face challenges such as limited land area, sensitivity to energy consumption, and high operational costs. Through system simulation and parameter optimization, we propose a decarbonization process using MDEA as the solvent, with controlled thermal load and a CH_4 recovery efficiency exceeding 97%. This offers a reusable design baseline for small- and medium-scale methane utilization systems, such as those in urban sewage treatment plants and kitchen waste gasification plants.

However, the current study has several inherent limitations. The simulation framework does not incorporate practical operational factors such as solvent aging, foaming, or real-world process fluctuations. Furthermore, the assumptions of ideal tray efficiency and simplified pressure drop may result in an overly optimistic performance assessment, underscoring the need for experimental validation to calibrate the model. Beyond these simplifications, the analysis does not explore advanced system integration measures,

including waste heat recovery or solvent formulation optimization. It is also recognized that the equilibrium-stage model represents a deliberate simplification suited for system-level screening. Future research should integrate rigorous kinetic models for the MDEA–CO_2 reaction system to support detailed column internals design and dynamic process analysis.

Future research will focus on the following directions: integrating compression waste heat with a heat pump coupled system to reduce the reboiler load, exploring alternative solvent systems such as activated MDEA formulations, and developing a multi-objective optimization framework to balance gas purity, energy consumption, and cost. Additionally, efforts will be made to integrate simulations with experimental data, enhancing the engineering adaptability and practicality of the research findings.

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