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Integrated Environmental, Economic, and Safety-based Optimization of Industrial Carbon Capture Process

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Abstract: Natural gas is a vital component of global energy supply. Methane (C1) is the chief component of natural gas, accounting for 80-85 mol% of its composition, with some other light alkanes present. In natural gas, other compounds in the mixture are undesirable because they contribute to corrosion, especially in piping systems and equipment, due to the gas's inherent water saturation. Moreover, the presence of CO_2 in natural gas prevents it from meeting the heating value requirement, thereby failing to meet the quality standards for natural gas. In this work, the carbon capture process in industry is multi-objectively optimized with respect to three objectives: environmental (global warming potential (GWP)), economic (return on investment (ROI)), and safety (damage index). In total, eight decision variables are considered, subject to two constraints related to CO_2 and H_2S concentrations. In the initial segment (from solution X to Y), the feed pressure increases by 53%, the feed gas temperature decreases by 29%, the reboiler pressure decreases by 38%, the feed molar flow decreases by 18%, and the lean amine temperature decreases by 27%. This rise in feed flow results in a significant increase in ROI to 46.9%.

Keywords: Carbon capture; NSGA-II; Promax; Optimization; Global warming potential.

1. Introduction

Natural gas (NG) is an indispensable fuel resource worldwide [1]. Methane (C1) is the primary component of NG, accounting for about 80-85 mol%, along with other light alkanes. Since natural gas originates from nature, it contains impurities in the form of H_2S, CO_2, carbonyl sulfide (COS), and mercaptans [1]. These undesirable impurities disrupt operations and have negative consequences, such as corrosion of pipelines and equipment, especially under frequently occurring water-saturated conditions. The presence of CO_2 in the exported gas reduces its calorific value, rendering it unable to meet quality criteria [2]. Therefore, NG needs to undergo certain treatment to meet sales criteria. Most national criteria require that H2S content be less than 4 ppm and that CO_2 levels not exceed 2 mol% [3]. The main challenge is then: which processes should be used to treat natural gas and meet sales criteria? Two important treatment processes include, first, a process for drying natural gas to avoid water saturation. Secondly, a carbon capture process that removes acid gases from the raw NG.

The industrial carbon capture process entails controlling and measuring multiple variables simultaneously to ensure uninterrupted operation. Variables such as temperature, pressure, and concentration need to be set to ensure the process is profitable and environmentally sustainable [4]. Optimization has proven useful in this case, enabling concurrent optimization of

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conflicting objective functions [5]. Prior examples of applying optimization techniques can be seen in various industries and complex processes [6-7]. Optimization has been successfully applied in the biochemical, chemical, oil and gas, polymers, waste treatment, biodiesel, and hydrogen production industries [8-10]. In this research, multi-objective optimization (MOO) is applied to the industrial carbon capture process, considering both environmental and economic objectives. The carbon capture process using amine-based solvents is a well-known and efficient method for capturing CO_2 emissions from oil and gas operations and power plants. Previous MOO research has optimized various gas-sweetening operations [1]. That MOO investigation employed Aspen Hysys and MATLAB environments. The novelty of the present work can be summarized as follows. The process simulation is built using Promax V6 software and validated using the industrial data [1]. Furthermore, the conflicting objective functions are included in the given case and solved using the NSGA-II evolutionary algorithm. The Pareto solutions are obtained, and their variation trend is justified through analysis of decision variables. The selected extreme solutions are compared and presented for further analysis.

2. Methodology

2.1 Process description

Referring to Fig. 1, sour gas containing acid gases enters the absorber column through its lower section. The absorber incorporates trays and a packed section positioned at the bottom of the column. Lean amine solvent, composed of MDEA, piperazine, and water, feeds into the absorber's top section, establishing counter-current contact between ascending sour gas and descending lean amine. Through this contact, acid gases transfer into the amine, producing sweet gas. Sweet gas exits from the absorber's upper portion and enters the amine wash water column's lower section. This four-tray column eliminates any amine solvent that may be entrained with the gas. Water accumulating at the bottom recirculates to the top of the column via the wash water pump, with a make-up system compensating for water losses. Treated sweet gas leaves the wash column and advances to downstream processing. Rich amine from the absorber, together with a minor liquid stream from the wash water column containing water and trace amine, flows to the rich amine flash vessel. This three-phase separator removes dissolved hydrocarbon gas and liquid, which are recycled back into the process. The degassed, rich amine is then filtered and preheated in a heat exchanger with lean amine before entering the regeneration column.

2.2 Problem formulation

After careful analysis of the process described in the section above, the decision variables are formulated. The process parameters, such as the temperature & pressure of the feed gas, the temperature & pressure of the regenerator, the concentrations of MDEA & Piperazine, the molar flow of the feed, and the temperature of the lean amine, are considered as decision variables in the current multi-objective optimization study. The lower and upper limits of the decision variables are selected after discussion with industry personnel. The details of the decision variables, constraints, and objectives are given in Table 1. The environment- and economy-based objective functions are formulated to account for their inherent conflict. In case 1, the global warming potential [3] objective function was formulated for minimization, while the return on investment (ROI) [1] was formulated for maximization. The objective of the damage index (DI) [1] is to be minimized. In case 2, the GWP and damage index objectives were optimized simultaneously. W-GWP is an important objective function that addresses environmental issues by minimizing greenhouse gas emissions. On the other hand, return on investment is an important factor to maximize, as it indicates how efficiently the investment is being used. Thus, two conflicting objective functions are formulated and optimized in this MOO study. A Promax-based model has been developed and combined with Excel Visual Basic, using a non-dominated sorting genetic algorithm (NSGA-II). The NSGA-II algorithm parameters used in this study are as follows: population size = 100; number of generations = 100; crossover probability = 0.8; and mutation probability = 0.03. The Penalty method for handling constraints is used. The NSGA-II algorithm is a widely used evolutionary algorithm. It has been used to address multi-objective optimization problems involving multiple conflicting objectives.

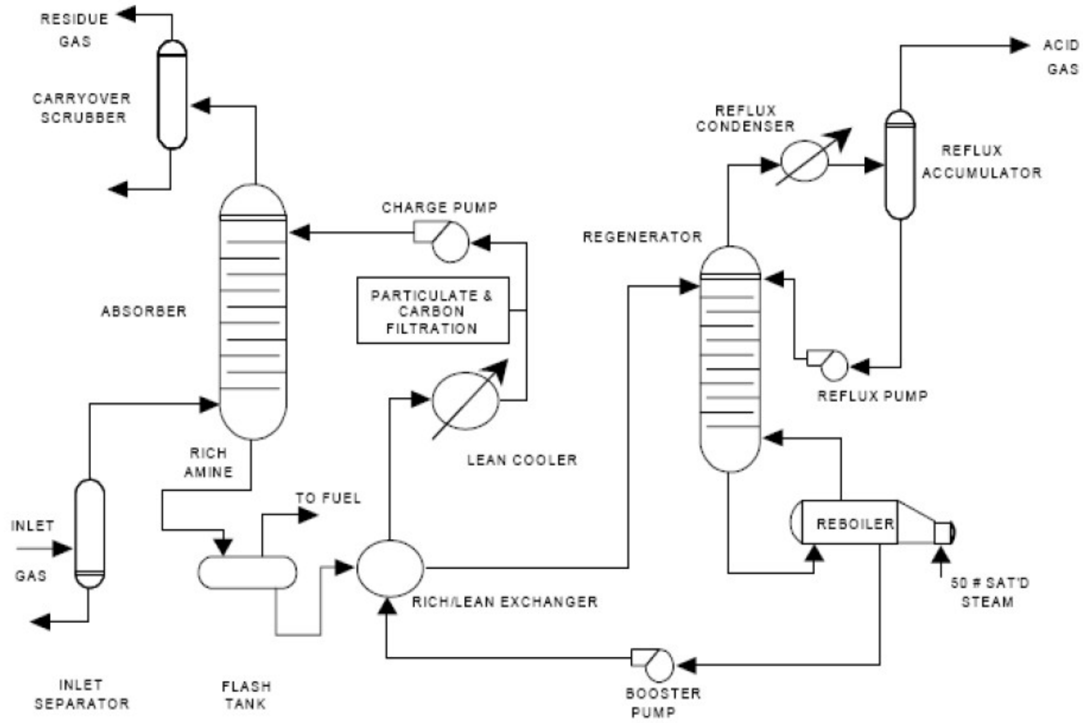

Figure 1. Typical carbon capture unit

Table 1. Details of design variables

Decision variables	Unit	Lower Limit	Upper Limit
Feed Gas Pressure (P_f)	kPa	4800	8000
Feed Gas Temperature (Tf)	°C	42	65
MDEA Concentration (Cm)	wt %	28	34.6
Piperazine Concentration (Cp)	wt %	2.9	5.8
Regenerator Pressure (Pr)	kPa	305	700
Regenerator Temperature (Tr)	°C	85	125
Feed Molar Flow (Mf)	kmol/hr	3000	4600
Lean Amine Temperature (Tla)	°C	50	72
Constraints	Concentrations: $H_2S \leq 4$ ppm and $CO_2 \leq 2$ mol%		
Objectives			
Case 1	W-GWP (mPE_{w94})		
	ROI (%)		
Case 2	W-GWP (mPE_{w94})		
	Damage Index		

3. Results and discussion

Case 1: Return on investment vs W-GWP

A multi-objective optimization investigation is conducted to minimize global warming potential (W-GWP) while maximizing return on investment (ROI), and the results are presented in this section. Process improvement, with its primary objective—acid gas removal—being critical in this context, should be connected to other objectives that deliver value from diverse perspectives, including economic, safety, and environmental considerations. Consequently, this discussion emphasizes improving two competing objective criteria. This MOO investigation focuses on resolving conflicts among objectives to determine Pareto-optimal solutions. Fig. 2(a) displays the Pareto-optimal solution for W-GWP minimization while maximizing ROI. Fig. 2(b-h) illustrates plots of design variables against the examined objective functions. According to Fig. 2(a), the trend of W-GWP minimization versus ROI maximization is divided into two intervals. During the first interval, spanning point X to point Y, return on investment rises sharply while W-GWP increases marginally. The second interval extends between points Y and Z, where ROI increases modestly while W-GWP escalates substantially. Table 2 summarizes objective function values and design variable values for the three solutions (X, Y, and Z) depicted in Fig. 2(a).

Table 2. Selected Points from the optimization study as shown in Fig. 2(a)

Objectives and Variables	Solution X	Solution Y	Solution Z
W-GWP (mPE_{w94})	11362.3	12076.8	16297.7
ROI (%)	21.3	31.3	34.3
Pf (kPa)	5154.3	7896.933	7999.629
Tf (°C)	63.3	44.649	45.3255
Cm (wt%)	34.3	33.957	34.572
Cp (wt%)	5.7	5.544	5.7285
Pr (kPa)	517.8	317.097	320.394
Tr (°C)	90	89.595	89.053
Mf (kmol/hr)	4499.6	3681.414	4522.5
Tla (°C)	69.9	50.886	50.853

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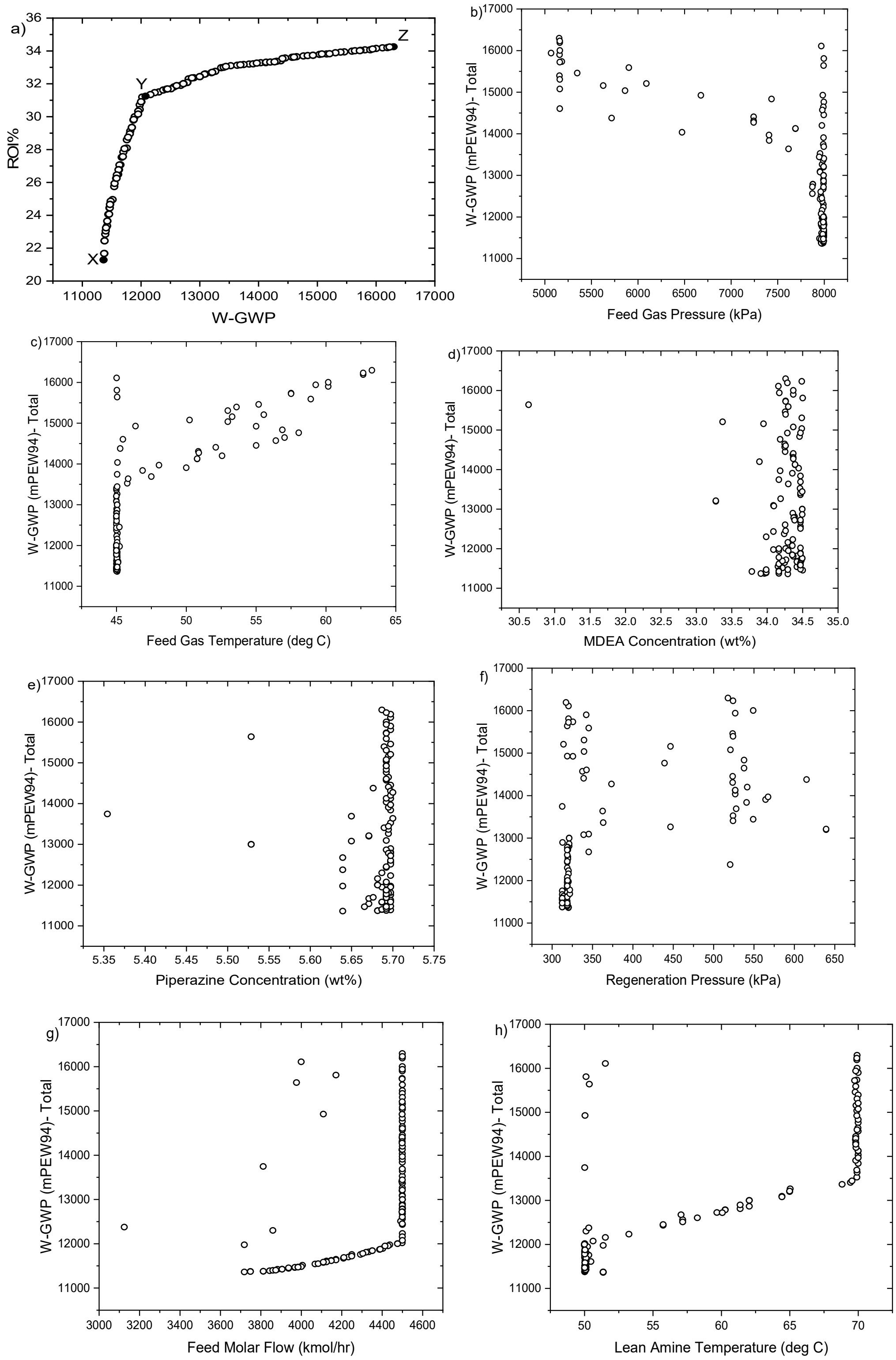

Figure 2. (a) Pareto optimal solutions, (b - h) variable trends

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In the initial segment (from solution X to Y), the feed pressure increases by 53%, the feed gas temperature decreases by 29%, the reboiler pressure decreases by 38%, the feed molar flow decreases by 18%, and the lean amine temperature decreases by 27%. This rise in feed flow results in a significant increase in ROI to 46.9%. This is reasonable since ROI is linked to profit, which in turn is dependent on product sales. Consequently, an increase in feed flow improves both the sales and, ultimately, the process's return on investment. In the subsequent segment (from solution Y to Z), the design variables that change include P_f, T_f, P_r, and T_{la}. Changes in the variables mentioned above led to a rapid rise in W-GWP. Conversely, the return on investment increased only marginally, which is not the intended outcome. Therefore, solution Y is regarded as the most favorable Pareto-optimal solution here, as it optimizes ROI to 46.9% while keeping W-GWP at 12076.8 mPE_{w94}.

Case 2: Damage Index vs % W-GWP

Multi-objective optimization of the damage index and global warming potential is performed to determine the operating conditions required for natural gas treatment. As we know, process safety is one of the most important factors to consider when operating any industrial plant, and it is important to determine the damage index, which indicates how safe the process is for the environment and workforce. W-GWP specifies the concentration of CO_2 absorbed, so if the concentration of the gas absorbed is higher, then W-GWP increases. From the MOO setup, we obtained the Pareto-optimal front and plots of the objective functions versus the decision variables.

From Fig. 3a, the plot of W-GWP versus damage index shows that reducing W-GWP increases the damage index. Although both objective functions were minimized, the trade-off showed that an increase in the damage index leads to a decrease in W-GWP. The damage index accounts for process conditions, usage limits, reaction conditions, etc., and process sacrifices must be made to reduce W-GWP, thereby increasing DI. W-GWP is highly important to reduce because of its long-term environmental impact, as it is one of the leading greenhouse gases contributing to global warming. From Fig. 3a, few scatter points at the start of the curve. The drop begins at a damage index of 587.5, corresponding to a W-GWP of 12282.27. As W-GWP decreases to below 11400, the damage index increases slightly above 620.

Fig. 3(b) shows the scattered solution points obtained from the MOO results for feed gas pressures between the upper and lower bounds. Fig. 3 (b) plots feed gas pressure in kPa and shows a distinctly bimodal distribution clustered near 5000 kPa and 8000 kPa, i.e., at both bounds. The feed gas temperature converged to 45 °C for most points, except for a few scattered points. A lower system temperature can lead to higher solvent absorption (Fig. 3(c)). MDEA concentration in the recycle stream, as shown in Fig. 3(d), for both objective functions converged mostly at the higher end of the concentration weightage, 34.5 wt.%. More solvent in the system means more absorption of the acid gases CO_2. Lean amine temperature converged to its lower bound of 50 °C (Fig. 3(h)). High lean amine temperatures can lead to ineffective performance of the absorber column and increase operating cost. Raising the temperature increases the risk of increased DI due to heat effects (Fig. 3(h)). Regeneration feed pressure ranges from 450 to 700 kPa (Fig. 3(f)). Regeneration temperature is kept low and converges at its lower limit of 85 °C. The PZ concentration in the amine recycle is scattered; however, the cluster is more towards the higher end, at 5.8 wt.% (Fig. 3(e)). Feed gas molar flow plays an important part. In Fig. 3(g), the feed gas molar flow data points range from 2400 kmol/hr to 3800 kmol/hr. There is a small trend that starts from approximately 3250 kmol/hr, where W-GWP decreases and the damage index increases. The W-GWP decrease can be classified as follows: increasing the flow rate increases pressure, which helps absorb the gases into the solvent. As such, the damage index also increases because a high gas flow rate results in higher pressure due to the greater amounts of gas and vapor present. DI is directly proportional to the feed gas molar flow rate; as plant capacity increases, the process equipment is utilized more effectively to meet proper process conditions, resulting in a higher DI.

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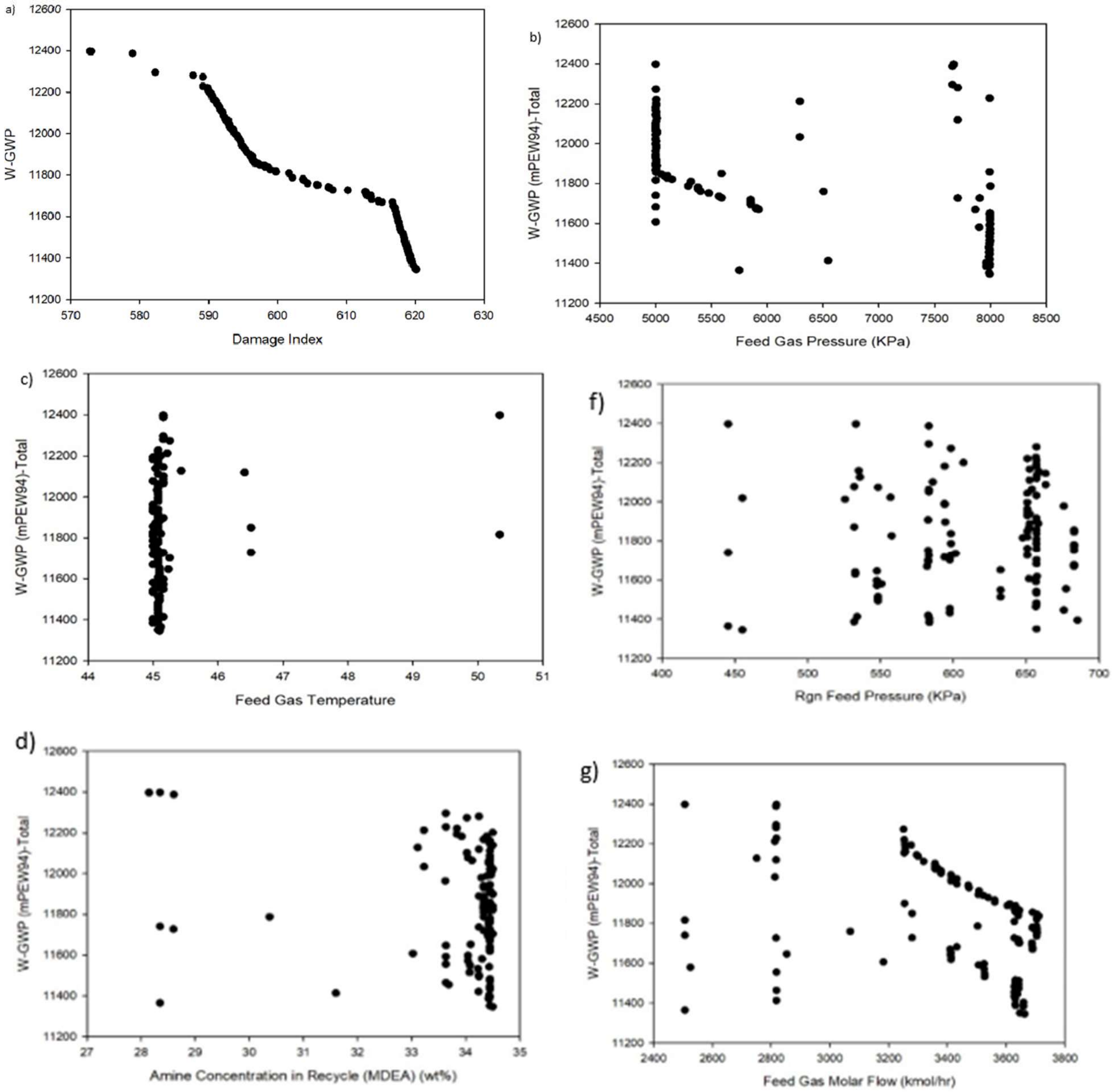

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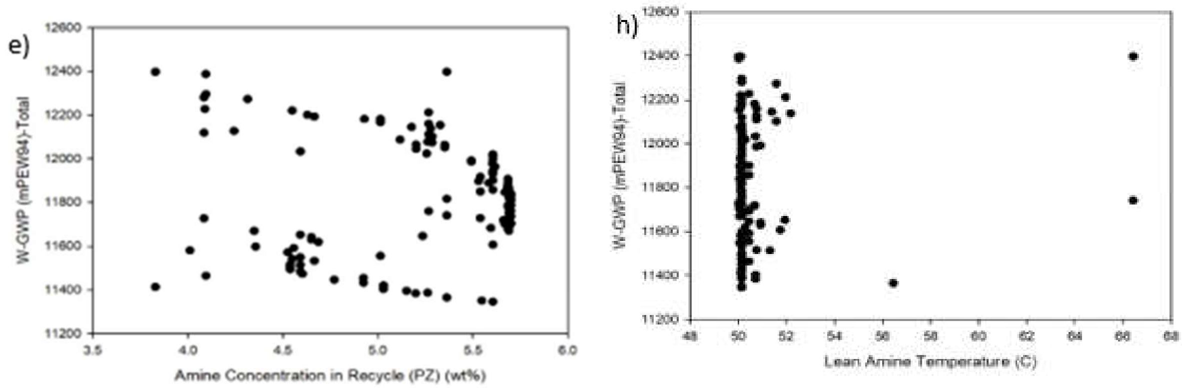

Figure 3: 3a Pareto Optimal front for W-GWP vs. damage index; 3b- 3h objective functions W-GWP versus decision variables

4. Conclusions

Natural gas sustainability and environmental impact depend substantially on the efficiency and cleanliness of processing and utilization. This industrial case study examines optimization of two competing objective functions: W-GWP minimization and ROI maximization. The most favorable Pareto-optimal solution resulted in an ROI of 46.9% and a W-GWP of 12076.8 mPE_{w94}. It was found that feed molar flow affects the ROI objective function more than it affects W-GWP. On the other hand, parameters such as absorber column operation and stripper column operation pressure impact W-GWP more than the ROI. Therefore, there is a need to optimize cleaner natural gas production. Consequently, the damage index (DI) also increases because a high gas flow rate results in higher pressure due to larger gas and vapor volumes. DI is directly linked to the feed gas molar flow rate; as plant capacity grows, the process equipment's maximum utilization also increases to meet required process conditions, causing DI to escalate.

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