

Multiobjective Optimization and Sustainability Assessment of an Improved Wet Sulfuric Acid-Based Ionic Liquid Process for the Utilization of Hydrogen Sulfide Using a Symmetry Approach

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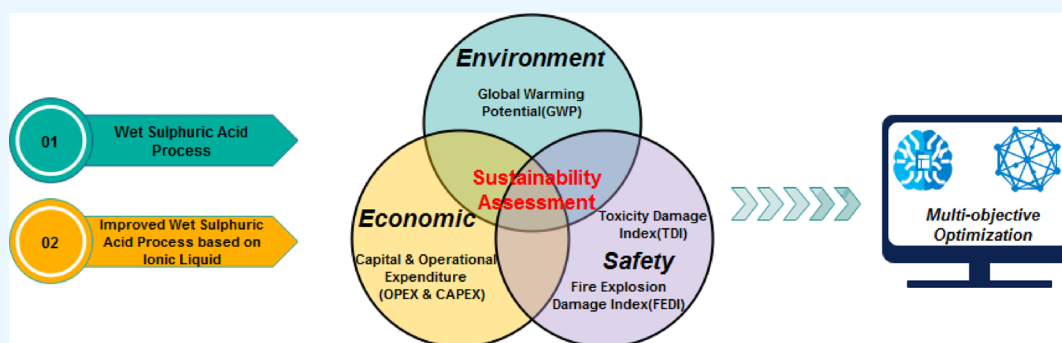


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ABSTRACT: Ionic liquids (ILs) are efficient media for the liquid-phase sulfuric acid reaction. Under mild situations, the reaction of H_2S with CH_4 in ILs happens extremely quick and virtually complete, resulting in liquid sulfuric acid ($\text{H}_2\text{SO}_{4(l)}$). 1-hexyl-3-methylimidazolium chloride ($[\text{hmim}][\text{Cl}]$) ILs were formerly the most effective at capturing and converting H_2S . It can convert H_2S to $\text{H}_2\text{SO}_{4(l)}$ with a proportion of up to 96%. This study aimed to develop cutting-edge techniques and assess their applicability for different acidic gas capacities and H_2S amounts by considering three sustainability metrics which are people (safety), planet (ecological), and profit. Then, to maximize profit while lowering the global warming potential (GWP), fire explosion damage index (FEDI), and toxicity damage index (TDI), a multiobjective optimization (MOO) case was performed. The trade-off between economic, environmental, and safety performance was expressed through Pareto-optimal solutions. The improved wet sulfuric acid (WSA)-based IL method was safer (lower fire and explosion damage index), ecologically friendly (lower GWP), and portable. The findings indicate that the improved WSA-based on IL gives the optimum results compared to conventional WSA processes, such as the profit of 5688\$/h increased from 1896\$/h, the GWP of 0.0138-ton CO_2 -eq decreased from 0.0275-ton CO_2 -eq, the TDI of 6.72 decreased from 13.44, and the FEDI of 6.18 decreased from 20.6, respectively. This discovery opens the door to a viable strategy for capturing and converting H_2S from an acid gas stream.

1. INTRODUCTION

Acid gas is a mixture that contains hydrogen sulfide (H_2S) and carbon dioxide (CO_2). Due to their acidic nature, both gases can cause significant damage to the industrial infrastructure and personnel. The presence of CO_2 and H_2S can cause stress, corrosion, and cracking of pipeline casings and tubing, resulting in catastrophic pipeline failure. Furthermore, H_2S is a poisonous gas that can cause eye irritation, coughing, nausea, and fatigue in the long run, even at low levels of exposure. H_2S is a frequently occurring pollutant in unprocessed natural gas produced from wells and petrochemical plants. Its concentration in fossil fuels differs widely across wells. It is colorless, poisonous, and highly flammable. It has a molar weight of 34 g/mol and a higher heating value of -60.3 °C. The reaction between H_2S and air is violent. It is a highly toxic gas that can corrode pipelines and other equipment. It is hazardous to the

environment and may endanger human health. Many fossil fuels containing H_2S are being emitted worldwide as the natural gas consumption rises. From 2010 to 2040, the entire usage of natural gas is predicted to rise at a rate of 20% per year.^{1,2}

Concerns about H_2S emissions from acid gas have recently shifted focus to developing alternative sulfur recovery technologies. Attempts are made to minimize emissions by converting H_2S into a competing entity. Sulfur recovery

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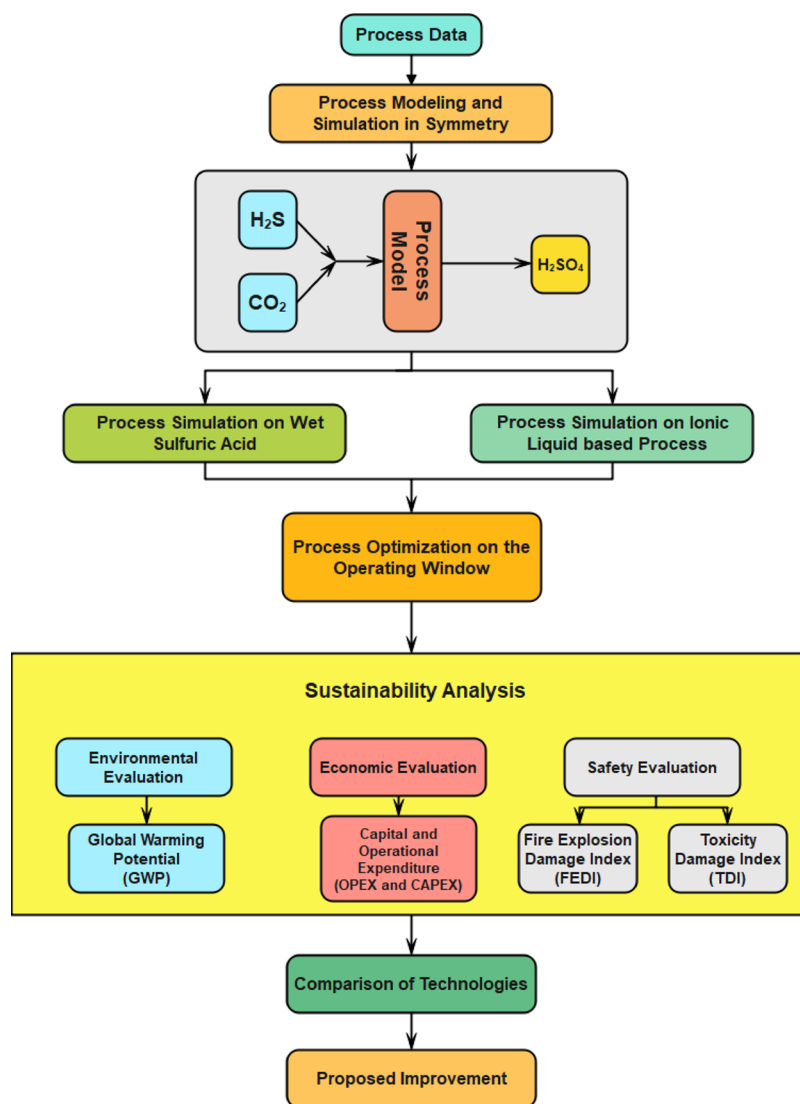


Figure 1. Overall methodology of the proposed framework.

technologies include the Claus and wet gas sulfuric acid processes.³ For decades, the Claus process has been used in the industry to convert H_2S to elemental sulfur. The bulk of this elemental sulfur is utilized to produce sulfuric acid. Wet sulfuric acid (WSA) provides an alternative method for directly converting H_2S into sulfuric acid. The WSA process is valuable for manufacturing sulfuric acid from acidic gas. From a sustainability perspective, it is critical to minimize H_2S emissions while generating a more valuable product in a healthier and more environmental friendly manner.^{4,5} In this respect, three crucial aspects of sustainability have been identified as the three pillars (Ps). The first pillar (“People”) implies a safer system. At the same time, “Planet” denotes a more ecologically friendly strategy, and “Profit” indicates that the method itself must generate a profit to be sustainable.

Acid gas has varying capacities and H_2S propositions despite these two cutting-edge technologies. This study aims to determine which of these two methods suits feed capacities and concentrations. The sustainability pillars are used to create accurate benchmarking metrics. Through a hazard and risk estimation analysis, the “People” pillar is suggested by well-known safety criteria such as fire explosion damage index (FEDI) and toxicity damage index (TDI), for assessing the

safety of the chemicals used and the process’s operating conditions. The global warming potential (GWP) is chosen as the environmental impact index for the “Planet” pillar.^{6,7} Finally, the process’s annual profit is used as the “Profit” pillar. Many studies have been conducted on optimization using a Symmetry simulation approach in conjunction with multi-objective optimization (MOO). For example, a MOO for different objective functions in the biodiesel production process was carried out using a modified version of the multiobjective differential evolution algorithm. They investigated the impact of various operational and design variables on process performance. They discovered that MOO has environmental and economic potential for this process, as they improved the conditions for maximizing profit and minimizing organic waste, among other goals. Flegiel created a MOO in Excel (EMOO).⁸ The investigated literature review on MOO of sulfuric acid plants reveals a lack of optimization of some essential environmental potentials, such as acidity potential (AP), GWP, and other critical economic objectives. A real-world sulfuric acid process plant model is validated in this study, and a MOO study is carried out with economic, environmental, and thermodynamic goals in mind.

The simulated model is developed with Symmetry simulation software and is used for MOO analysis in Excel with Visual Basic for application-based interface and optimization (EMOO) aspects.⁹ This is the first MOO study for an H₂SO₄ process plant for the objectives under consideration to our knowledge. However, evaluation processes solely based on economic performance may not provide a comprehensive picture or a sustainable process. In this regard, there are currently ongoing concerns about safety and environmental issues that must be addressed concurrently. These three objective functions (profitability, safety, and the environment) frequently clash. As a result, trade-offs are required in the design and selection process, particularly in the section of H₂S utilization technologies. There are currently some approaches to evaluate chemical processes that consider the profitability, safety, and environmental aspects.^{7,10,11}

Nonetheless, MOO research on H₂S usage methods is still sparse. As a result, there is a need to research and build a unique optimization platform that considers MOO while evaluating current commercial H₂S usage methods and comparing them to an ionic liquid (IL) technology.^{12,13} There is also a requirement to understand the process operating windows for these processes to answer issues such as which technology is more economically profitable, at which capacities, and within which concentration of H₂S. Understanding the influence of technology on space constraints (for example, offshore versus onshore) is equally critical.^{1,14,15}

Annual profit is assessed using technoeconomic assessment (TEA), while global warming potential (GWP) is measured using life cycle assessment (LCA). Moreover, FEDI and TDI, both classed as hazard potential, are solved using Khan et al.⁷ The objective is to discover the ideal circumstances while considering financial, ecological, and safety issues. The development problem is presented as a MOO challenge that must be addressed by a multiobjective genetic algorithm. It identifies optimal feed capacity, sulfuric acid allocation, and profit with the least amount of GWP and danger level. The results reflect the trade-off between the objectives.¹⁷

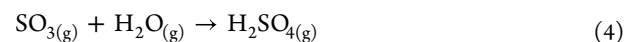
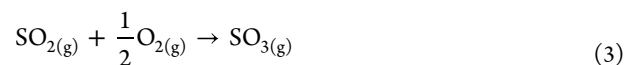
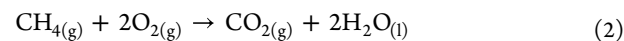
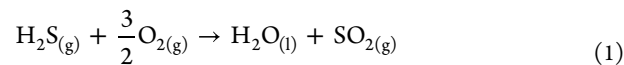
The rest of the article is organized as follows. Section 2 helps explain the methodology which is based on three pillars 1. Profit, 2. Environment safety and 3. Health hazard along with MOO. Section 3 concentrates on the results obtained from two case studies: 1. Conventional WSA process and 2. WSA process based on ionic liquids (ILs) after which comes the conclusion in Section 4.

2. METHODOLOGY

Figure 1 illustrates the proposed framework for this study and research, which included modeling and simulation of the WSA processes and the ionic liquid-based process in calculating TDI, FEDI, GWP, and yearly profit. First, process data can be extracted according to standard operating conditions in Symmetry simulation.

2.1. Wet Sulfuric Acid. The chemicals utilized in the simulations were hydrogen sulfide (H₂S), carbon dioxide (CO₂), carbon monoxide (CO), water (H₂O), methane (CH₄), sulfur dioxide (SO₂), sulfur trioxide (SO₃), nitrogen (N₂), oxygen (O₂), hydrogen (H₂), sulfuric acid (H₂SO₄), and elemental sulfur. Conversion reactors, heat exchangers, and separator vessels were typical unit operations employed in this simulation. The condenser in the WSA process served three primary functions. First, it was a location to react (converting SO₃ to H₂SO₄), second to reduce temperature and condense

SO₃ and H₂SO₄, and thirdly separate liquid H₂SO₄ and clean gas. There is no WSA condenser unit in Symmetry package that can do these three operations.^{18–20} As a result, a conversion reactor, heat exchanger, and vessel were employed to replicate a single WSA condenser.



The central composite design (CCD) approach was used to vary the H₂S proposition and input gas feed capacity in this project, as indicated in Table 1. This strategy was utilized to

Table 1. Feed Capacity and % Concentration of H₂S

run	feed capacity (kgmol/h)	H ₂ S concentration in mole %
1	64.4	2.64
2	64.4	52.3
3	198.80	2.64
4	198.80	52.3
5	108.9	23.15
6	82.4	5.28
7	82.4	62.89
8	228.3	5.28
9	228.3	62.89
10	198.80	10.575

reduce the number of simulations runs required while allowing for enough variability to generate appropriate regression models for the WSA and improved WSA techniques.

Regression models in Symmetry was used to perform simulation due to its fast substantially computations as compared to other software packages. The findings of each simulation were then used to create the indices mentioned above reflecting (3Ps) that provided more information on calculating FEDI, TDI, GWP, and yearly profit.^{21,22}

The regression models were created based on feed capacity (X₁) and H₂S concentration (X₂). In this study, a generic version of a second-order regression model was applied. It is depicted below.

$$Y = aX_1 + bX_2 + cX_1^2 + dX_2^2 + eX_1X_2 + f \quad (6)$$

As a result, four models were created for each WSA and ionic liquid-based process. As previously stated, the dependent variables (Y) are TDI, FEDI, GWP, and yearly profit. The literature contains further information on the process and the subsequent outcomes.

2.2. Process Based on IL. The advent of ILs provides an excellent opportunity to overcome the issues encountered in gas treatment. ILs are a type of organic molten salt with melting points close to or below room temperature. Their distinct qualities, such as exceptionally low volatility, great thermal stability, and excellent affinity with acidic gases, meet the general requirements of promising gas separation media.^{23–27} Most crucially, we may modify the IL framework to specific needs. ILs have been demonstrated to be excellent

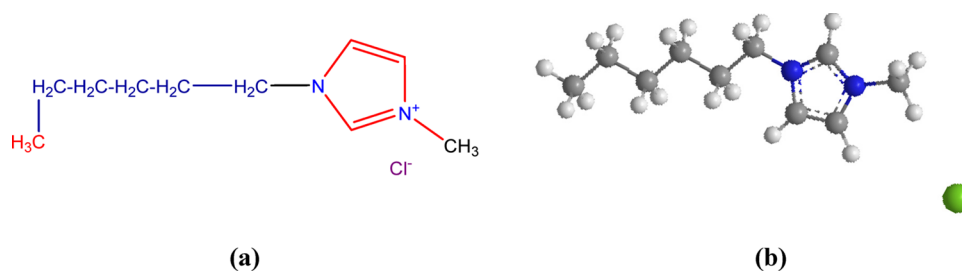


Figure 2. (a) Structural and (b) 3-D representation of ([hmim][Cl]) IL.

solvents for the selective absorption of H_2S and SO_2 . These findings encourage us to investigate the idea of employing ILs as a medium for the capture and conversion of H_2S via the WSA process. Although the absorption–desorption process has long been recognized as a key strategy to sour gas treatment, integrated capture–conversion will be more promising green chemistry.²⁶ A WSA process mediated by ILs is described in this paper. 1-Hexyl-3-methylimidazolium chloride ([hmim][Cl]) IL was formerly the most effective at capturing and converting H_2S . It can convert H_2S to $\text{H}_2\text{SO}_4(l)$ with a proportion of up to 96%. It is discovered that the interaction of H_2S with SO_2 occurs very quickly and thoroughly in the IL phase, resulting in element sulfur. Figure 2 depicts the collection and conversion of H_2S in ILs via the WSA process. In a sealed reaction chamber, the IL was presaturated with SO_2 , and then stoichiometric H_2S was delivered into the chamber. To track the course of the reaction, the pressure in the reaction chamber was monitored online. There are two stages during the capture and conversion of H_2S : first, H_2S in the gas phase is transferred into the IL phase, and then H_2S combines with SO_2 in the IL phase to produce sulfuric acid and water. Our modeling and designing strategy involve the preuse of the IL.¹⁶ Figure 2 presents the structural and 3-D representation of ([hmim][Cl]) IL.

Although ILs have minimal vapor pressures, the resulting sulfur-bound salts would emit no foul odors. Unlike the situations documented in the literature, these ILs can mole maximum scavenging H_2S and thiols.²⁸ Figure 3 illustrates a simple chemical strategy used to create such ILs.

2.3. Sustainability Assessment on the Moving Windows Approach. For the initial model of the conven-

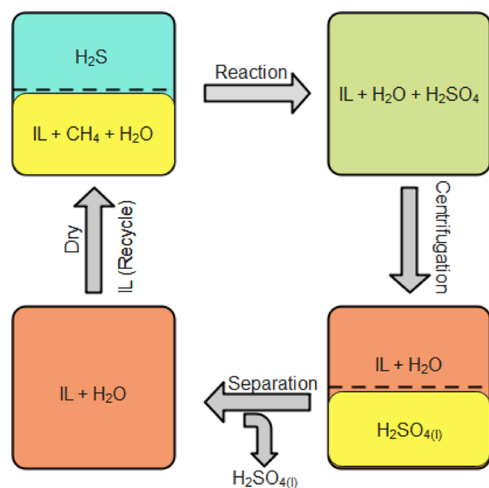


Figure 3. Improved WSA-based IL process.

tional WSA and improved process based on the IL, the annual profit, GWP, and hazard potential in terms of FEDI and TDI were utilized to estimate the optimum values. These various requirements result in a MOO issue in which the yearly profit must be maximized while the GWP, FEDI, and HIRA are minimized.²⁹ Feed capacity and product yields are the decision factors, whereas mass and energy balances, as well as the global product demand, are the constraints. Prior to dealing with MOO concerns, the developed process simulation models are simplified as surrogate models that link decision elements to objectives. Regression models are created using rigorous simulation findings acquired via a CCD to address the MOO issue later. MOO issues create optimal results, indicating the trade-off between the objectives.³

2.3.1. Environmental Evaluation. The integrated bio refinery environmental impact assessment employs the LCA technique following ISO standards. The developed process simulation includes all emissions, including direct emissions from the process, power, and heat consumption. The scope of this work lies on the utilization of IL (ionic liquid) to get the optimum results. Eq 7 indicates that the total life cycle inventory (LCI) may be calculated based on direct emissions, energy use, and heat demand.

$$LCI_{\text{tot}} = LCI^{\text{process}} + LCI^{\text{electricity}} + LCI^{\text{heat}} \quad (7)$$

After that, the LCI is converted into a GWP. (CO_2), (CH_4), and (NO_x) are these gases considered (N_2O). As stated in eqs 8 and 9, the GWP is calculated by adding the GWPs from these other sources.

$$GWP = \sum_i LCI_{\text{tot}} \times m_i \quad (8)$$

$$GWP_{\text{tot}} = \sum_j GWP_j + \sum_k GWP_k \quad (9)$$

In this equation, m_i is the damage factor attributable for each greenhouse effect, which is derived from Guinee.³⁰ GWP_j represented the pretreatment process of GWP, while GWP_k denotes the GWP in the chemical manufacturing process.

2.3.2. Economics Evaluation. Symmetry is used to calculate the TEA of the processes. The simulated outcomes and equipment sizing are used to make this estimate. The investment components from eqs 10 to 12 are used to calculate the project capital expenditure for the yearly operational cost estimate.³¹ Yearly profit is evaluated as the difference between yearly product sales and total operating cost, which is the sum of (CAPEX) and (OPEX). As indicated in eqs 10–12, the economic goal is to maximize annual profit (\$/year).

$$\text{Profit} = \sum_m B_m^{\text{prod}} C_m^{\text{prod}} - \sum_j \sum_k C_{a_{jk}} - \sum_j \sum_k O_{p_{jk}} \quad (10)$$

$$C_a = \sum_j \sum_k T_{dc} + T_{idc} + C_{fe} + C_{on} + F_{ci} \quad (11)$$

$$O_p = \sum_j \sum_k D_{mc_{st}} + F_{mc_{st}} + G_{mc_{st}} \quad (12)$$

The mass production rate of products is given by B_m^{prod} (kg/h), while the product price is given by C_m^{prod} (\$/kg). The annual CAPEX for the pretreatment and final procedures is (\$/year). CAPEX covers the whole direct and indirect plant costs and the contractor fee, contingencies, and development costs. The total of direct, fixed, and general manufacturing costs equals (\$/year).

2.3.3. Inherent Safety Evaluation. FEDI and TDI are two hazardous potentials that have been quantified in this study. The energy factor is the key part of the computation in FEDI, which depends on thermodynamic statics. Another consideration is the penalty, determined by the process operating range. Storage units, physical, chemical reactions sections, transportation units, and other hazardous sections are all subject to fines. Finally, multiplying the penalty and energy components results in the FEDI damage potential. The most significant part of TDI computation is the processing unit contains a potentially dangerous product.^{5,32} The physical and chemical process are evaluated consequently. They are frequently issued for the origin of the next hazardous section and the area utilized by the section due to a malfunction of relevant data collected during the product development stage; eqs 13–22 indicate how FEDI and TDI were computed.

$$F_1 = 0.1M \times \frac{Hc}{K} \quad (13)$$

$$F_2 = 1.304 \times 10^{-3} \times P_p \times V \quad (14)$$

$$F_3 = 1 \times 10^{-3} \times \frac{1}{(T + 273)} \times (P_p - V_p)^2 \times V \quad (15)$$

$$F_4 = M \times \frac{Hr \times n}{K} \quad (16)$$

$$D_p = (F_1 \times p_{n_1} + F_2 + p_{n_4} + F_4 \times p_{n_7}) \times p_{n_3} \times p_{n_4} \quad (17)$$

$$\text{FEDI} = 4.76(D_p)^{1/3} \quad (18)$$

$$G = A \times m \quad (19)$$

$$\text{TDI} = a(G \times p_{n_1} \times p_{n_2} \times p_{n_3} \times p_{n_4})^b \quad (20)$$

$$\text{FEDI}_{\text{total}} = \sum_j \text{FEDI}_j + \sum_k \text{FEDI}_k \quad (21)$$

$$\text{TDI}_{\text{total}} = \sum_j \text{TDI}_j + \sum_k \text{TDI}_k \quad (22)$$

TDI denotes the chemical volumetric flow rate (m³/h) has a G factor as well as a number of penalties. The G factor is computed from A, and m is the predicted mass flowrate in kg/s.

2.4. Multiobjective Optimization. The WSA and ionic liquid-based processes are optimized using a multiobjective approach that considers economic, environmental, and thermodynamic goals.^{33,34} Evolutionary algorithms are readily accessible. Several choice factors (pressure and raw material flow rates) are considered at the operational level since they significantly impact the targeted optimization objectives.^{7,35} Acid purity, SO₂ permitted emissions, reactor output temperature, and water content in air are also restricted. Two environmental targets, GWP and AP, are proposed for optimization, together with economic assessment objectives such as utilization cost \$/year (UT), fixed capital investment (FCI), production cost \$/year (PRS), and total production cost (TPC).

$$\text{Normalized GWP} = \frac{\text{GWP}}{\text{Norm. ref.}_{\text{GWP}}} \quad (23)$$

$$\text{Weighted GWP} = W_{\text{FGWP}} \times \text{Normalized GWP} \quad (24)$$

where normalization GWP is the normalized global warming potential of the substance under consideration, which in this case is carbon dioxide. WFGWP is the global warming weighting factor while eqs 25 and 26 are utilized for AP calculations.

$$EF_i = \frac{n}{MW_i} \times 32.03 \quad (25)$$

$$\text{AP} = \sum_i EF \times m_i \quad (26)$$

The molecular weight of the substance emitted is MW_i, the number of hydrogen ions released is n, and the equivalence factor is EFi.³⁵ Carbon dioxide is the sole component of this sulfuric acid manufacturing facility that contributes to GWP, but H₂SO₄, SO₃, and SO₂ contribute to rising AP.³⁶ The exergy calculation technique is simplified by utilizing the equations, but the economic-based targets such as FCI (based on bare module cost) were computed using the equations and correlations provided by refs 11 and 37. The utility costs for power, steam, and cooling water, among other things, were calculated, while TPC includes utility costs in addition to raw material costs such as water and sulfur, as stated in eq 27:

$$\text{TPC} = \text{UT} + \text{RM} + \text{Other expenses} \quad (27)$$

Other costs include labour-related activities, maintenance, operational overhead, depreciation, and so on. Other expenditures are calculated as a proportion of PRS or FCI using this approach. Sulfur costs \$60 per ton, electrical energy costs 0.062 cents per kWh, water costs 0.0015 cents per liter, sulfuric acid costs \$200 per ton, steam costs 0.001 cents per kilogram, and cooling water costs 0.354 cents per gallon.¹⁶

3. RESULTS AND DISCUSSION

In the period leading up to MOO, each process was subjected to a sustainability assessment to determine its economical profit, process safety, and environmental influence. These findings are illustrated in Tables 2 and 3 and Figure 3 in the additional data. This work investigates two MOO cases. As shown in Table 6, there are two bi-objective cases (maximizing yearly profit and minimizing GWP, maximizing yearly profit, and minimizing hazard potentials) and one triobjective instance (maximizing yearly profit and minimizing GWP FEDI, and TDI). In all instances, the constraints that have

Table 2. Combustor Feed Parameters of the WSA Process

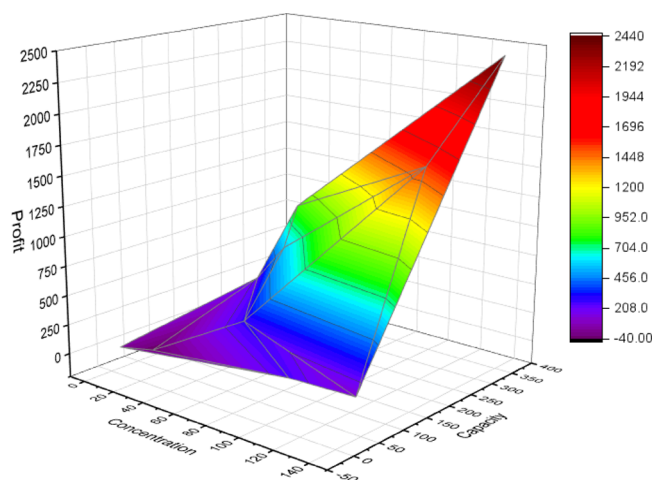
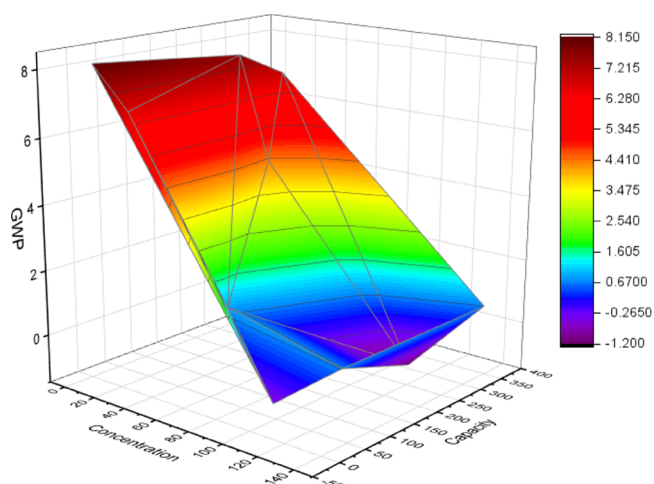
stream no	temperature (°C)	pressure (kPa)	flowrate (kgmol/h)
acid feed	35	210	250
air feed	45	210	550

Table 3. Process Parameters of the WSA Process

run	capacity (X_1)	concentration (X_2)	X_1^2	X_2^2	X_1X_2
1	0.4914	6.435	0.24147396	41.40923	3.162159
2	0.4914	113.4	0.24147396	12859.56	55.72476
3	279.6	6.435	78176.16	41.40923	1799.226
4	279.6	113.4	78176.16	12859.56	31706.64
5	107.76	52.5225	11612.2176	2758.613	5659.825
6	43.956	12.75	1932.12994	162.5625	560.439
7	43.956	138.6	1932.12994	19209.96	6092.302
8	350.712	12.75	122998.907	162.5625	4471.578
9	350.712	138.6	122998.907	19209.96	48608.68
10	279.6	25.05	78176.16	627.5025	7003.98

been considered are applied. In the case of tri objective optimization, one optimal solution is chosen from among the nondominated solutions because it addresses all 3Ps of sustainability. The MOO stage was derived from the Symmetry approach,³⁸ and the multicriteria statement tool was the MS Office application software (Figure 4).³⁹

3.1. Case Study 1: Minimize Hazard Potential, Minimize Environmental Impact, and Maximize Profit Conventional Wet Sulfuric Acid. The optimal outcome for Case 1 MOO is shown in Figures 5 and 6. The x-axis represents the concentration, the y-axis shows (annual profit/GWP/TDI/FEDI), and the z-axis shows feed capacity. Each optimal coordination shows the optimum WSA superstructure design with a novel trade-off of yearly profit, GWP, TDI, and FEDI. Three Pareto-optimal solutions are chosen as optimum solution samples for further investigation. Profit data variables for the regression model in the WSA process are shown in Table 4, and GWP data variables for the regression model in the WSA process are shown in Table 5; TDI data variables for the regression model in the WSA process are shown in Table 6,

**Figure 5. Regression model of profit in the WSA process.****Figure 6. Regression model of GWP in the WSA process.**

and FEDI data variables for the regression model in the WSA process are shown in Table 7.

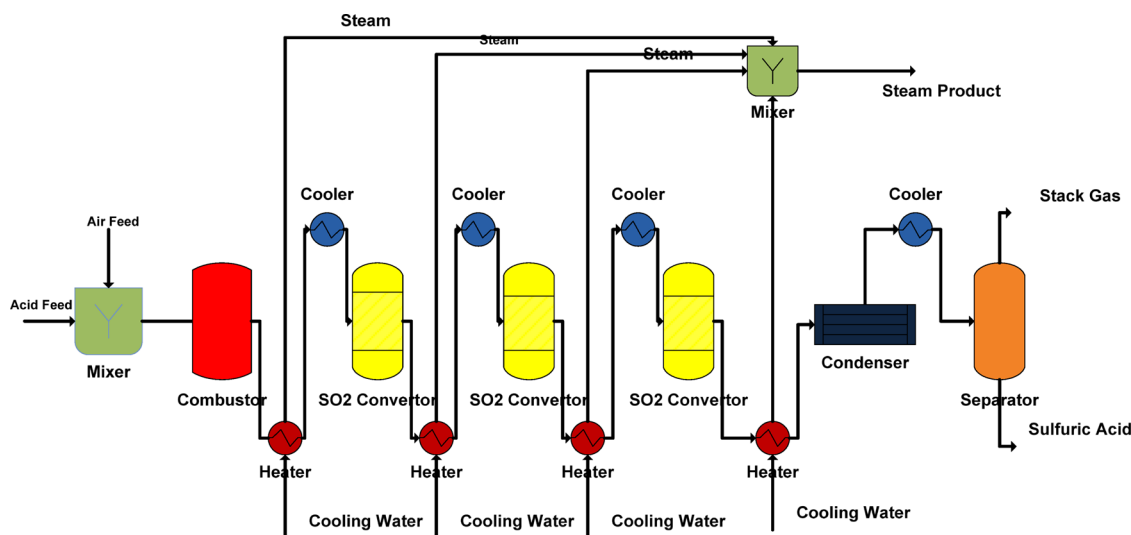
**Figure 4. WSA process simulation diagram.**

Table 4. Profit Data Variables for the Regression Model in the WSA Process

run	profit (\$/h) simulation	profit (\$/h) model
1	0	39.12
2	0	244.155
3	0	216.765
4	1287	1544.025
5	363.048	271.515
6	58.344	-38.13
7	233.04	124.53
8	911.4	823.14
9	1896.06	2436.93
10	233.4	565.59

Table 5. GWP Data Variables for the Regression Model in the WSA Process

run	GWP simulation	GWP model
1	7.668	8.145
2	0.108	-0.45
3	7.668	7.605
4	0.192	-1.17
5	0.624	0.825
6	3.6456	6.645
7	0.0276	0.69
8	5.064	6.87
9	0.0276	0.66
10	2.2752	4.35

$$Y = -4.332X_1 + 10.49X_2 + 0.016X_1^2 - 0.072X_2^2 + 0.037X_1X_2 - 23.3599 \quad (28)$$

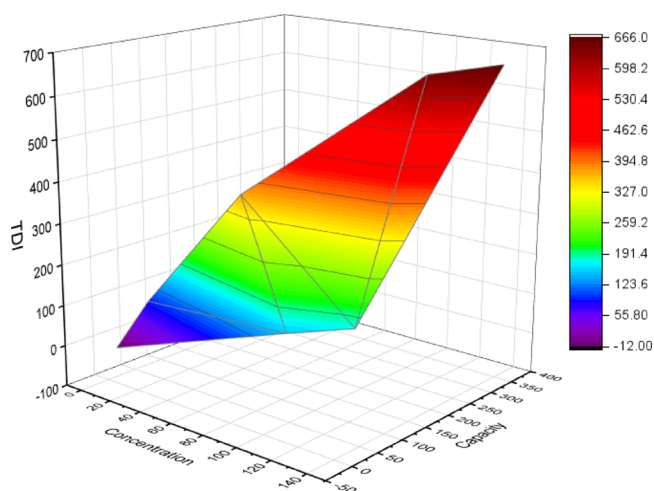
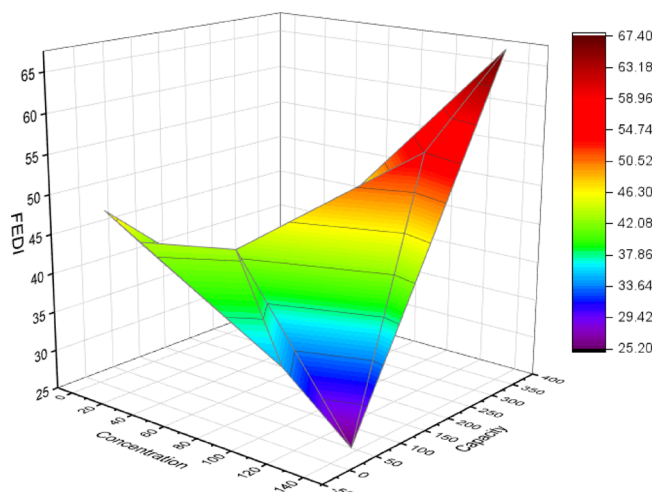
Table 6. TDI Data Variables for the Regression Model in the WSA Process

run	TDI simulation	TDI model
1	13.44	-10.73
2	34.88	152.92
3	16.41	144.57
4	646.12	642.91
5	438.19	368.26
6	89.41	92.99
7	262.46	172.31
8	262.67	152.14
9	641.04	664.2258
10	278.66	303.6772

Table 7. FEDI Data Variables for the Regression Model in the WSA Process

run	FEDI simulation	FEDI model
1	49.728	47.835
2	20.616	34.605
3	20.616	29.655
4	50.58	54.795
5	37.788	42.945
6	25.02	43.2
7	25.308	25.335
8	32.892	35.565
9	48.684	67.305
10	27.492	37.905

Figure 5 shows the effect of H₂S concentrations and feed capacity on the profit of WSA. Interestingly, the profit increases with decreased environmental impact. Profit should ideally be increased while the GWP is minimized. Furthermore, as seen in the Pareto-optimal front (POF), the excellent efficiency of one objective function (OF) comes from the price of inferior performance of the other. As a result, Figures 7 and 8 show an ideal description, each equally desirable for TDI and FEDI.

**Figure 7. Regression model of TDI in the WSA process.****Figure 8. Regression model of FEDI in the WSA process.**

The sulfuric acid production in Figure 5 ranges from 1750 to 2440 \$/h and has the maximum yearly profit and shows a decrease in GWP, TDI, and FEDI. The feed capacity supply and process concentration are maximized in this system, as is the mass allocation to produce sulfuric acid (70%). It outperforms economic and environmental effects due to reduced capital investment and yearly production costs, greater product profit, and inferior GWP value. The same is valid for increasing sulfuric acid production due to increased worldwide demand. It depicts the WSA configuration of the red solution point with 100 tons/h of H₂SO₄ given to the process that increases the yield of H₂SO₄ supplied to the plant.

A range from 700 to 1700 \$/h is an in-between option in which a slight decline in plant feed capacity (99 ton/h) results

in increased plant profit. The similar WSA design yearly profit is 905 M USD/year and 283-ton CO₂-eq, respectively. As the maximum value 2440 \$/h indicates, the maximum H₂S is utilized to make sulfuric acid. Finally, the 0–1000 \$/h is the lowest profit range. Profit will be higher by increasing feed capacity. As a result, more feed capacity supply must be coordinated to maximize profit, causing a logistical problem within the facility.

The wet sulfuric acid process shows the lowest profit 58.344 \$/h at 43.95 kmol/h and 12.75 mol % and the highest profit of 1896 \$/h at 350 kmol/h and 138.6 mol %. Hence it is concluded that if feed capacity increases, profit also increases.

$$Y = -0.00839X_1 - 0.2066X_2 + 2.33 \times 10^{-5}X_1^2 + 0.00105X_2^2 - 6.4 \times 10^{-6}X_1X_2 + 9.43508 \quad (29)$$

The wet sulfuric acid process shows the lowest global warming potential at higher concentration 138.6 mol % and higher feed capacity 350.7 kmol/h and show higher GWP at 0.491 kmol/h and 6.435 mol/h. Hence it is concluded that at higher feed capacity, the concentration of GWP is low.

$$Y = 1.5463X_1 + 6.7986X_2 - 0.00379X_1^2 - 0.044X_2^2 + 0.01121X_1X_2 - 53.4564 \quad (30)$$

The wet sulfuric acid process shows a higher toxic damage index at higher feed capacity 279 kmol/h and concentration 113.4 mol %, and show the lowest TDI at the lowest feed capacity 0.491 kmol/h and concentration 6.435 mol %. Hence Figure 7 indicates that at the lowest feed capacity, the concentration of TDI is also low.

$$Y = -0.15188X_1 + 0.7578X_2 + 0.00028X_1^2 - 0.00235X_2^2 + 0.001285X_1X_2 + 46.98632 \quad (31)$$

3.2. Case Study 2: Minimize Hazard Potential, Minimize Environmental Impact, and Maximize Profit on Improved Wet Sulfuric Acid Process Based on ILS. The Pareto-optimal solutions for the improved WSA-based IL process case of objective optimization are shown in Figures 9–12. The x-axis represents the concentration of H₂S, the y-axis shows (annual profit/GWP/TDI/FEDI), and the z-axis shows feed capacity. Compared to conventional WSA, the

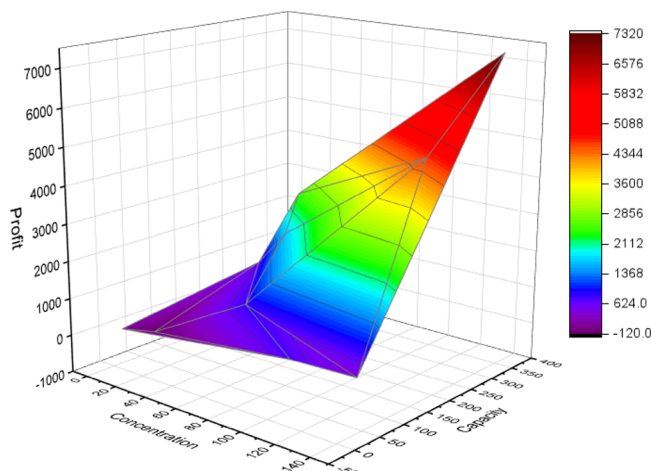


Figure 9. Improved regression model of profit in the WSA-based IL process.

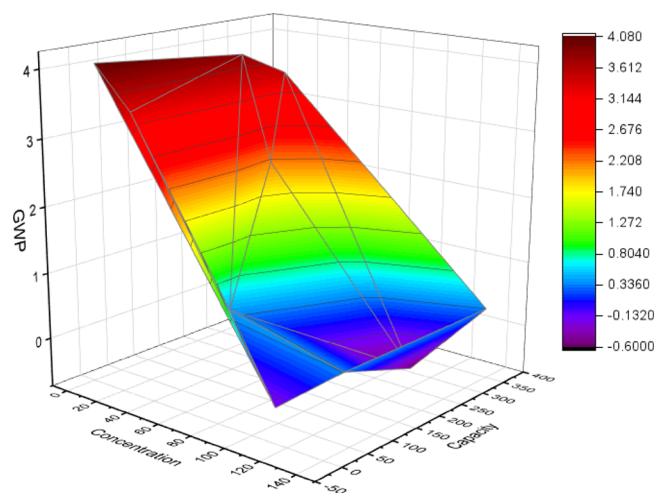


Figure 10. Improved regression model of GWP in the WSA-based IL process.

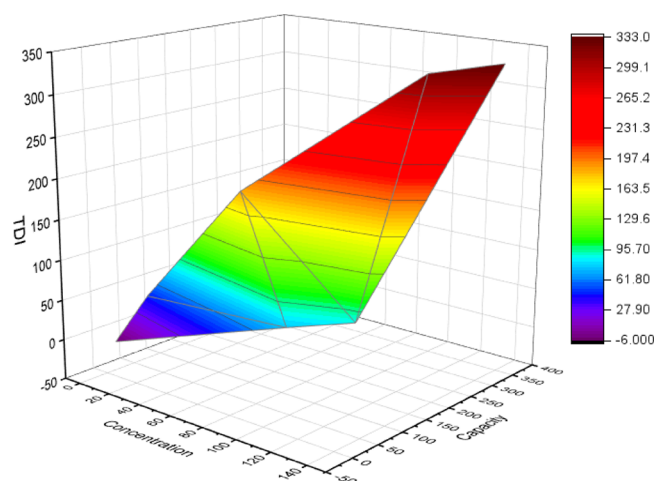


Figure 11. Improved regression model of TDI in the WSA-based IL process.

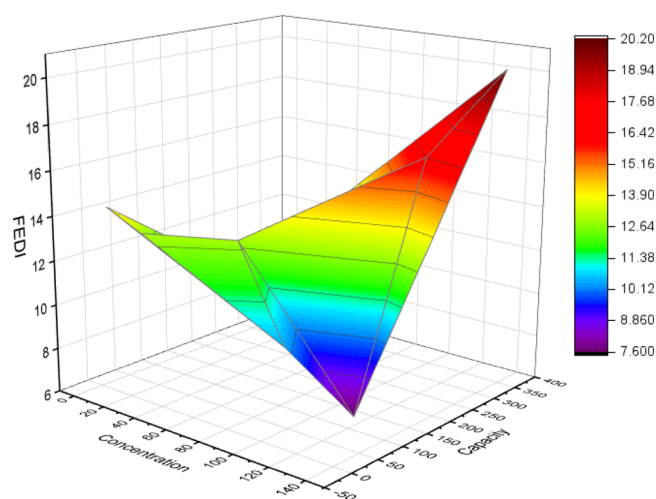


Figure 12. Improved regression model of FEDI in the WSA-based IL process.

improved WSA gives the optimum results. Each Pareto-optimal point represents the optimum WSA superstructure design with a unique trade-off of yearly profit, GWP, TDI, and

FEDI. Three Pareto-optimal solutions are chosen as optimum solution samples for further investigation. Figure 9 shows the effect of H₂S concentrations and feed capacity on the profit of improved WSA. Interestingly, the profit increases with decreased environmental impact. The profit should ideally be increased while the value of GWP is diminished. Nevertheless, as shown in the POF, the better effectiveness of OF comes at the disbursement of the worse performance of others. As a result, Figures 9 and 10 show an ideal description, each equally desirable for TDI and FEDI.

The sulfuric acid production in Figure 9 ranges from 5000 to 7000 \$/h and has the maximum yearly profit with decreases in GWP, TDI, and FEDI. The feed capacity supply and process concentration are maximized in this system, as is the mass allocation to produce sulfuric acid (85%). It outperforms economic and environmental effects due to reduced capital investment and yearly production costs, more significant production profit and selling price, and an inferior GWP value. The same scenario is valid for increasing sulfuric acid production due to increased worldwide demand. It depicts the WSA setup of red solution points with 100 tons/h of H₂SO₄ delivered to the chemical process, corresponding to the maximum H₂SO₄ supplied to the plant.

A range from 2200 to 4200 \$/h is an intermediate option in which a modest drop in feed capacity (99 ton/h) outcomes in an increase in profit. The yearly profit and GWP of the equivalent WSA design are 907 M USD/year and 286-ton CO₂-eq, respectively. As the maximum value 7000 \$/h indicates that maximum H₂S is utilized to make sulfuric acid. Finally, the 0–2000 \$/h is the lowest profit range. Profit and environmental effects are both higher with somewhat more feed capacity. As a result, more feed capacity supply trucks must be coordinated to maximize profit, causing a logistical problem within the facility. Profit data variables for the regression model in the WSA-based IL process shown in Table 8, GWP data variables for the regression model in the WSA-

Table 8. Improved Profit Data Variables for the Regression Model in the WSA-Based IL Process

run	profit (\$/h) simulation	profit (\$/h) model
1	0	117.36
2	0	732.465
3	0	650.295
4	3861	4632.075
5	1089.144	814.545
6	175.032	-114.39
7	699.12	373.59
8	2734.2	2469.42
9	5688.18	7310.79
10	700.2	1696.77

based IL process shown in Table 9, TDI data variables for the regression model in the WSA-based IL process shown in Table 10, and FEDI data variables for the regression model in the WSA-based IL process shown in Table 11.

$$Y = -12.998X_1 + 31.45703X_2 + 0.0506X_1^2 - 0.21498X_2^2 + 0.112768X_1X_2 - 70.1698 \quad (32)$$

The wet sulfuric acid-based IL process shows the lowest profit 699 \$/h at 43.95 kmol/h and 138 mol % and the highest

Table 9. Improved GWP Data Variables for the Regression Model in the WSA-Based IL Process

run	GWP simulation	GWP model
1	3.834	4.0725
2	0.054	-0.225
3	3.834	3.8025
4	0.096	-0.585
5	0.312	0.4125
6	1.8228	3.3225
7	0.0138	0.345
8	2.532	3.435
9	0.0138	0.33
10	1.1376	2.175

Table 10. Improved TDI Data Variables for the Regression Model in the WSA-Based IL Process

run	TDI simulation	TDI model
1	6.72	-5.365
2	17.44	76.46
3	8.205	72.285
4	323.06	321.455
5	219.095	184.13
6	44.705	46.495
7	131.23	86.155
8	131.335	76.07
9	320.52	332.1129
10	139.33	151.8386

Table 11. Improved FEDI Data Variables for the Regression Model in the WSA-Based IL Process

run	FEDI simulation	FEDI model
1	14.9184	14.3505
2	6.1848	10.3815
3	6.1848	8.8965
4	15.174	16.4385
5	11.3364	12.8835
6	7.506	12.96
7	7.5924	7.6005
8	9.8676	10.6695
9	14.6052	20.1915
10	8.2476	11.3715

profit of 1896 \$/h at 350 kmol/h and 138.6 mol %. Hence it is concluded that if feed capacity increases, profit also increases.

$$Y = -0.00441X_1 - 0.10364X_2 + 1.21 \times 10^{-5}X_1^2 + 0.000529X_2^2 - 5.9 \times 10^{-1}X_1X_2 + 4.727295 \quad (33)$$

The wet sulfuric acid-based IL process shows the lowest global warming potential at the higher concentration 138.6 mol % and lower feed capacity 43.95 kmol/h and show a higher GWP at 0.491 kmol/h and 6.435 mol/h. Hence it is concluded that at higher feed capacity, the concentration of GWP is low.

$$Y = 0.7731X_1 + 3.39932X_2 - 0.0019X_1^2 - 0.02201X_2^2 + 0.005605X_1X_2 - 26.7282 \quad (34)$$

The wet sulfuric acid-based IL process shows a higher toxic damage index at higher feed capacity 279 kmol/h and concentration 113.4 mol %, and shows the lowest TDI at the lowest feed capacity 0.491 kmol/h and concentration 6.435

mol %. Hence Figure 11 indicates that at the lowest feed capacity, the concentration of TDI is also low.

$$Y = -0.04556X_1 + 0.047346X_2 + 8.41 \times 10^{-5}X_1^2 - 0.00071X_2^2 + 0.000386X_1X_2 + 14.0959 \quad (35)$$

The wet sulfuric acid-based IL process shows a higher fire and explosion damage index at lower feed capacity 0.491 kmol/h and concentration 6.435 mol % and shows a lower FEDI at lower feed capacity 0.491 kmol/h and higher concentration 113 mol %. Hence Figure 12 indicates a lower FEDI at a lower feed capacity and higher concentration.

4. CONCLUSIONS

This work demonstrates efficient H₂S collection and conversion in IL using an improved WSA reaction. In a simple IL, 1-hexyl-3-methylimidazolium chloride ([hmim][Cl]), H₂S can be converted to sulfuric acid with an excellent one-stage conversion ratio of 96.4%. IL can be utilized several times without losing activity. It developed two MOO cases, first with profit maximization, and second for GWP, FEDI, and TDI minimization. The resulting mass and energy balances were then utilized to evaluate the appropriateness of these processes at varied input gas feed capacity and H₂S concentrations. As comparative measures, three pillars of sustainability were used: people (safety), planet (environment), and profit. A number of simulations runs in Symmetry are used to get more comprehensive results. Regression models were created from selective simulation runs by using the CCD to do efficiently. The results show that the improved WSA-based on IL gives the optimum results compared to conventional WSA processes. The improved WSA process is the most sustainable technology for H₂S conversion at the same concentrations and feed capacity ranges. Furthermore, the WSA method is more convenient and efficient, generating a rise in profit and lowering the GWP, FEDI, and TDI index such that the profit is increased from 1896 to 5688\$/h, the GWP decreased from 0.0275-ton CO₂-eq to 0.0138-ton CO₂-eq, the TDI decreased from 13.44 to 6.72, and the FEDI decreased from 20.6 to 6.18, respectively.

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Notes

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