COMPARATIVE STUDY OF SULFUR REMOVAL USING SOLVENT SOLUTIONS: AMINES, HYBRIDS, AND SELEXOL™ SOLVENT

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ABSTRACT

Environmental limits on sulfur components and concerns regarding sulfur poisoning of catalysts require removal of these components to a range from 15 mg/m^3 to 150 mg/m^3 depending on downstream operations. The challenge lies in determining which technology provides optimal results on key process parameters that will impact CAPEX and OPEX.

The effectiveness of sulfur removal from natural gas streams using solvent technology depends on the interplay between solvent chemistry and process requirements. Mercaptans, due to their low polarity and acidity, are not efficiently removed by conventional amine solvents, which are better suited for more acidic species like H_2S. In contrast, physical solvents excel at achieving deep mercaptan removal, but their strong affinity for hydrocarbons can lead to significant co-absorption, impacting product recovery and necessitating additional capital investment for separation. Advanced solvent formulations, including hybrid solvents that blend chemical and physical absorption mechanisms, offer a pathway to optimize total sulfur removal by balancing energy consumption, hydrocarbon losses, and equipment sizing. Selecting the most suitable solvent system requires a clear understanding of process specifications and identification of the limiting sulfur species, enabling operators to minimize circulation rates, energy demand, and capital expenditures while meeting stringent environmental and product quality standards.

This work employs a systematic methodology to quantitatively compare different solvent technologies for total sulfur removal across a spectrum of operating conditions. Multiple case scenarios are analyzed, encompassing variations in acid gas composition and product specifications, to assess the operational performance and process suitability of each solvent system. Our proprietary simulation tool (ProComp 10) is utilized to predict removal of sulfur components with each of the solvent technologies. The simulation prediction is compared with the performance of hybrid solvent based on actual plant data, highlighting the simulator accuracy and reliability in real-world applications.

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Introduction

Effective removal of sulfur components from natural gas streams is an essential aspect of gas processing to meet product specifications and maintain environmental compliance. With increasingly stringent regulations and pipeline standards worldwide, the industry has explored more efficient and cost-effective approaches for achieving low sulfur content in final products. The need for sulfur removal has grown due to several factors. Regulatory agencies around the world have reduced permissible sulfur limits in pipelines and product specifications, driven by environmental and public health objectives. Sulfur components present in natural gas and NGL products can cause toxicity, corrosion and, when combusted, produce sulfur oxides (SO_x), which contribute to air pollution, acid rain, and respiratory issues [1-3]. Catalyst poisoning by sulfur is another concerning factor. Trace sulfur compounds, such as hydrogen sulfide (H_2S) and mercaptans, can attach to the catalyst's active sites and form sulfides that hinder reactions. As a result, downstream processes like hydro-processing and reforming become less efficient [4]. To avoid these issues, thorough upstream sulfur removal is necessary.

Technologies for removing sulfur from natural gas include chemical and physical solvent processes, direct oxidation, molecular sieves, and catalytic hydrolysis. Each method offers distinct advantages and limitations. Direct oxidation, exemplified by the Merox process, is often used for selective mercaptan removal, particularly in liquid hydrocarbons, but may be adapted for gases. The process converts mercaptans to disulfides with a catalyst and air, featuring moderate capital and operating costs and mild conditions. It produces limited waste but is less effective for COS removal and less suitable for high concentrations of mercaptans or sour gases due to catalyst fouling and oxygen management challenges [2]. Molecular sieve technology enables deep removal of mercaptans, COS, water, and other sulfur components. Zeolite-based sieves are effective for trace contaminant removal under strict specifications [3]. A key advantage is consistent achievement of sub-ppm sulfur levels, although this technology incurs higher operating costs due to thermal regeneration needs and sensitivity to heavy hydrocarbon contamination. High initial investment and complexity of operation are additional considerations. Catalytic hydrolysis is commonly employed for COS removal, converting COS to H_2S over catalysts such as alumina or titanium-based materials in the presence of water vapor. The converted H_2S can then be removed using standard amine processes. This technique is highly selective for COS and integrates efficiently with acid gas removal systems, but effectiveness relies on precise temperature and moisture control, and catalyst deactivation by contaminants requires ongoing maintenance [5].

For decades, solvents have been the primary method for removing acid gases from diverse gas streams, offering efficient and thorough sulfur removal in a single step while minimizing waste and energy use. Various gas-treating solvents—such as amine-based, physical, and hybrid formulations—are available to meet the wide-ranging demands of sulfur removal in natural gas processing. Each solvent technology possesses unique characteristics and delivers operational benefits tailored to specific process requirements:

- UCARSOL™ AP series of solvents, hereafter referred to as aqueous amine-based solvents, efficiently remove CO_2 and H_2S via chemical absorption but are inefficient for mercaptan removal. Therefore, standard gas treating units using amine solvents typically require multiple steps or a very high solvent flowrate to achieve total sulfur removal, accounting for various sulfur species [3, 6, 7].
- SELEXOL™ Solvents, hereafter referred to as physical solvents exhibit a strong affinity for organic sulfur components, including mercaptans. Its performance is driven by physical absorption rather than chemical reaction, making it particularly effective for removing weakly acidic species like mercaptans. This solvent has a high affinity towards H_2S and shows relatively limited capacity towards COS [3]. Physical solvents are generally preferred when the gas stream contains relatively low levels of heavy hydrocarbons, which otherwise would get co-absorbed and lost via the acid gas.
- UCARSOL™ Hybrid series of solvents, hereafter referred to as hybrid solvents, enable total sulfur removal in a single treatment step. These solvents combine physical and chemical absorption properties, making it possible to treat complex gas streams with mixed sulfur compositions, while controlling co-absorption of hydrocarbons compared to pure physical solvent [5]. The application of hybrid systems in operational facilities validates the potential benefits in simplifying processes, eliminating the need for a secondary acid gas recovery unit, thus achieving cost savings. Hybrid solvents in combination with advanced operation schemes are becoming increasingly prominent due to enhanced flexibility and the potential for operational simplification. Technology selection depends on feed gas composition, target product specifications, utility constraints, financial factors, and other site-specific requirements.

This study presents a comparison of solvent technologies under diverse operating conditions and offers a practical framework for selecting the most suitable solvent for total sulfur removal. Various scenarios are analyzed to assess the performance and applicability of these technologies across different sour gas compositions. Additionally, plant data will be provided to validate prediction accuracy using our proprietary gas processing simulation tool, ProComp10.

Methodology

Five distinct cases derived from actual customer inquiries were evaluated. These cases were categorized into separate groups based on their defining characteristics and application contexts. The feed gas composition and concentration for all these cases are presented in **Table 1**. The specification of the treated gas is <10 ppmv of total sulfur components.

Case 1: The scenario termed low acid gas refers to a feed gas with all major acid gas components: hydrogen sulfide (H_2S), carbon dioxide (CO_2), mercaptans, and carbonyl sulfide (COS).

Case 2: The moderate acid gas scenario involves a feed containing increased levels of H_2S and CO_2, while the concentrations of mercaptans and COS are unchanged from Case 1. This case investigates how higher levels of H_2S and CO_2 affect solvent selection and system performance.

Case 3: This scenario describes a feed gas with substantially elevated acid gas concentrations, predominantly H_2S, referred to as high acid gas.

Case 4: This case addresses the removal of mercaptans from molecular sieve regeneration gas streams (regen-gas case), which generally have high mercaptan concentrations.

Case 5: This case examines a feed gas containing trace amounts of acid gases, mercaptans, and COS. In this scenario, unit sizing is primarily influenced by the presence of mercaptans and COS.

Table 1 – Feed Gas Dry Composition for All Cases

Component	Unit	Case 1	Case 2	Case 3	Case 4	Case 5
CO_2	mol %	2.0	6.0	2.0	6.43	0.98
H_2S	mol % (ppmv)	2.0	5.0	18.0	0.0005 (5)	0.004 (40)
Methyl Mercaptan	ppmv	100	100	100	700	16
Ethyl Mercaptan	ppmv	80	80	80	-	-
Propyl Mercaptan	ppmv	20	20	20	-	-
Butyl Mercaptan	ppmv	10	10	10	-	-
COS	ppmv	100	100	100	-	21
N_2	mol %	7.86	7.85	1.34	0.85	7.83
CO	mol %	0.41	0.41	-	-	0.41
CH_4	mol %	67.74	60.75	62.87	89.69	70.79
C_2H_6	mol %	13.27	13.27	9.33	1.94	13.27
C_3H_8	mol %	3.86	3.86	3.97	0.65	3.86
nC_4H_{10}	mol %	1.38	1.3800	1.74	0.18	1.38
nC_5H_{12}	mol %	0.86	0.86	0.49	0.09	0.86
nC_6H_{14}	mol %	0.62	0.62	0.26	0.17	0.62

The feed gas conditions for this study are standardized at 100°F (37.8°C), 800 psig (55.2 barg), and a flow rate of 100 MMSCFD (at 60°F and 1 atm) for all cases except Case 4. In Case 4, the objective is to assess sulfur removal from regeneration gas at 77°F (25°C), 950 psig (65.5 barg), and a flow rate of 100 MMSCFD. Different feed gas compositions under different case scenarios were investigated in which heavy hydrocarbons, C_6+, are not included in these case studies. The treated gas specification is also fixed, aiming for total sulfur components of 10 ppmv. The study aims to identify optimal strategies for sulfur removal under diverse feed compositions, highlighting trade-offs in efficiency and cost. In this study, the standard process scheme is employed as shown in **Figure 1** for all solvent technologies to be identical in terms of process configurations for the purpose of this comparative study. The absorber column was configured with three sections, each containing 20 ft (6.1 m) of 4th generation 2-inch (50 mm) random packing. Similarly, the regenerator column was designed with two 20 ft (6.1 m) sections of 4th generation 2-inch (50 mm) random packing. For simulating the Lean-Rich Heat Exchanger (LRHX), a heat transfer coefficient of 420 BTU/[hr·ft^2·°F] (2380 W/[m^2·K]) was applied.

Sulfur removal using amine-based (50 wt.% non-H_2O), physical (97 wt.% non- H_2O), and hybrid (75-80 wt.% non-H_2O) solvents was investigated to understand the performance of each of these solvents at gas processing plants. The effects of different solvent technologies on process variables such as reboiler duty, solvent circulation rates, LRHX size and duty, and lean cooler duty were explored.

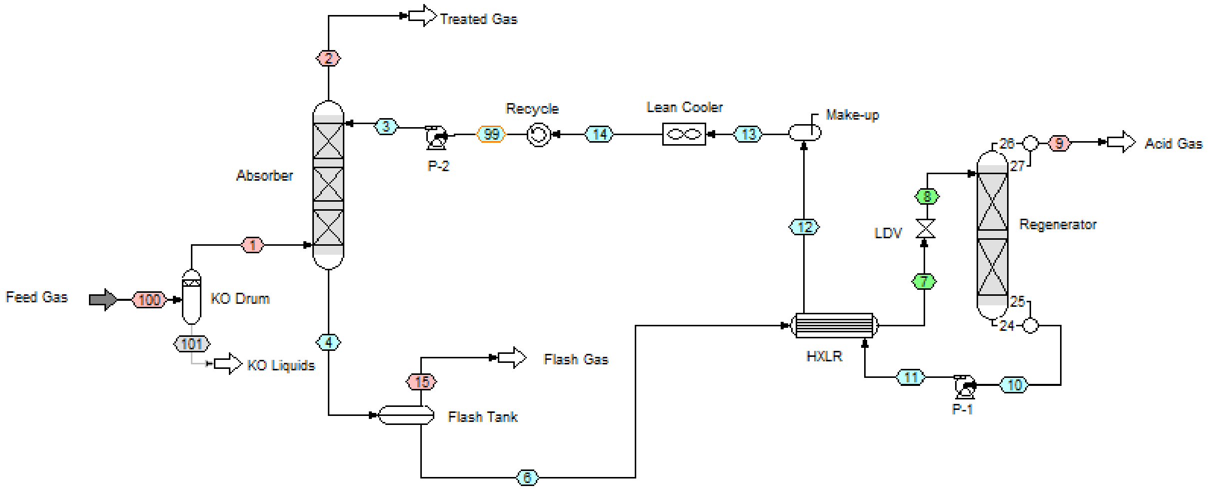

Figure 1 – ProComp10 Process Flow Diagram

Results And Discussion

Case 1: Low Acid Gas

Comparative results using physical and hybrid solvents are presented in **Table 2**. Performance of each solvent was independently optimized, aiming for minimum solvent circulation rate and reboiler duty.

The comparison between physical and hybrid solvents revealed distinct performance and operational differences. The hybrid solvent achieved a lower COS concentration in treated gas (3.5 ppmv vs. 9.6 ppmv), while the physical solvent is significantly more effective in removing mercaptans. **Table 3** shows the relative solubility of sulfur components in the physical solvent compared to methane, indicating the physical solvent has a strong affinity towards methyl mercaptan but a moderate affinity towards COS. The hybrid solvent, on the other hand, can remove COS by chemical bonding and achieve a tighter COS specification if needed.

Table 2 – Simulation Results Using Hybrid and Physical Solvents for Case 1

Parameter	**Physical Solvent**	**Hybrid Solvent**
COS concentration in treated gas (ppmv)	9.6	3.5
H_2S concentration in treated gas (ppmv)	<1.0	1.6
Mercaptan concentration in treated gas (ppmv)	<1.0	3.7
Solvent flowrate, USgal/min (m^3/hr)	954 (217)	788 (179)
LRHX duty, MMBtu/hr (Gcal/hr)	48.2 (12.1)	19.7 (4.97)
Lean cooler duty, MMBtu/hr (Gcal/hr)	−17.3 (−4.36)	−20.3 (−5.11)
Condenser duty, MMBtu/hr (Gcal/hr)	−7.02 (−1.77)	−10.2 (−2.56)
Reboiler duty, MMBtu/hr (Gcal/hr)	17.9 (4.51)	33.4 (8.41)
Absorber diameter, ft (m)	6.74 (2.05)	6.78 (2.07)
Regenerator diameter, ft (m)	5.05 (1.53)	6.07 (1.85)
Methane recovery (%)	97.1	99.4
Ethane recovery (%)	90.0	98.3
Propane recovery (%)	82.1	97.5
Butane recovery (%)	56.2	96.3
Pentane recovery (%)	23.2	94.3
Hexane recovery (%)	1.8	87.5

The hybrid solvent requires less solvent circulation rate but demands more energy in the regenerator reboiler and condenser. The regenerator diameter in the hybrid design is larger, 6.07 ft compared to 5.05 ft in the physical solvent design, as more steam is required to strip acid gas components from the solvent. The chemical bonds between the hybrid solvent and acid gases demand more energy for regeneration.

As shown in **Table 3**, hydrocarbons exhibit significant solubility in the physical solvent, with their affinity increasing proportionally to hydrocarbon molecular weight. Solubility of hydrocarbons in the hybrid solvent is significantly lower, resulting in noticeably higher hydrocarbon recoveries across all components, especially for heavier hydrocarbons like hexane and pentane.

Notably, the physical solvent uses a chiller for its lean cooler, which requires an extra cooling duty and requires higher solvent flow rates even at low lean temperatures. This flow rate will be substantially higher if an air cooler is used instead of the chiller. Overall, the hybrid solvent offers superior recovery and efficiency.

Since the affinity of COS in the physical solvent is lower compared to H_2S and mercaptans, an alternate design scenario was developed based on Case 1 gas composition but excluding COS from the feed gas and the sulfur removal requirement. **Table 4** offers insight into how each solvent performs when COS is absent, helping to isolate the impact of this component on overall sulfur removal efficiency.

With the removal of COS from the feed, the required circulation rate to meet product specifications was found to be lower when using the physical solvent compared to the hybrid solvent system. This reduction in flow contributed to a smaller regenerator diameter in the physical solvent design.

These findings highlight the efficiency of physical solvents in minimizing equipment sizing and operational demands under comparable conditions for cases in which there is no COS in feed gas. If the customer is concerned about hydrocarbon recoveries, a hybrid configuration would be a more suitable option; however, it will come at the expense of increasing regeneration duty requirements. It is noteworthy that both reboiler energy consumption and lean cooler duty are lower for the physical solvents in this scenario. Additionally, the limiting component differs between the two processes: in the physical solvent configuration, H_2S acts as the controlling species, whereas in the hybrid process, the constraint shifts to mercaptan removal.

Table 3 – Relative Solubility of Gas Components in SELEXOL Solvents [3]

Component	**R= K`[1] component/K` CH_4**
CH_4	1
C_2H_6	7.20
C_3H_8	15.4
C_4H_{10}	36
C_5H_{12}	83
C_6H_{14}	167
CO_2	15.2
COS	35
H_2S	134
CH_3SH	340

Table 4 – Simulation Results Using Hybrid and Physical Solvents for Case 1 Alternate

Parameter	**Physical Solvent**	**Hybrid Solvent**
H_2S concentration in treated gas (ppmv)	9.6	<1.0
Mercaptan concentration in treated gas (ppmv)	<1.0	9.0
Solvent flowrate, USgal/min (m^3/hr)	765 (174)	776 (176)
LRHX duty, MMBtu/hr (Gcal/hr)	40.0 (10.1)	19.3 (4.88)
Lean cooler duty, MMBtu/hr (Gcal/hr)	−12.3 (−3.09)	−20.1 (−5.06)
Condenser duty, MMBtu/hr (Gcal/hr)	−8.94 (−2.25)	−9.89 (−2.49)
Reboiler duty, MMBtu/hr (Gcal/hr)	14.8 (3.73)	32.9 (8.29)
Absorber diameter, ft (m)	6.49 (1.98)	6.74 (2.06)
Regenerator diameter, ft (m)	4.54 (1.38)	6.04 (1.84)
Methane recovery (%)	97.6	99.5
Ethane recovery (%)	92.2	98.6
Propane recovery (%)	86.0	98.1
Butane recovery (%)	68.1	97.5
Pentane recovery (%)	41.3	95.4
Hexane recovery (%)	7.66	91.1

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[1] K`=y/x where y is the mole fraction of the component in the vapor phase and x is the mole fraction of the component in the liquid phase considering only the solvent and the component.

Case 2: Moderate Acid Gas

The comparative results for physical and hybrid solvents are presented in **Table 5**. Both solvents were evaluated under identical design conditions to assess their performance in acid gas removal and hydrocarbon recovery. The hybrid solvent achieved a significant reduction in CO_2 concentration in the treated gas, lowering it to < 1 ppmv, compared to 4.9 mol % for physical solvent. Due to a relatively high CO_2 concentration in the feed, the hybrid solvent requires a higher solvent circulation rate (1350 USgal/min) than the physical solvent (986 USgal/min) to maintain process efficiency and meet the required treated gas total sulfur specification. Essentially, the physical solvent benefits from its ability in slipping CO_2, while the hybrid solvent removes most of CO_2.

The physical solvent system operates using solvent refrigeration with an estimated duty of −16.2 MMBtu/hr, and the hybrid solvent requires an air cooler duty of −37.7 MMBtu/hr to reach the required lean solvent temperature of 40°F (4.4°C) and 120°F (48.9°C), respectively. The techno-economic analysis needs to be done to estimate the cost implications of a larger air cooler required for the hybrid solvent compared to solvent refrigeration required for the physical solvent system. The hybrid's higher reboiler duty and increased circulation rate necessitate larger absorber and regenerator towers. Consequently, the regenerator reboiler duty for the hybrid (57.3 MMBtu/hr) is significantly higher than that for the physical solvent (20.1 MMBtu/hr), reflecting greater energy consumption. Despite higher energy and cooling requirements, the hybrid solvent delivers superior hydrocarbon recovery across all components.

Table 5 – Simulation Results Using Hybrid and Physical Solvents for Case 2

Parameter	Physical Solvent	Hybrid Solvent
CO_2 concentration in treated gas (ppmv)	48600	0.6
COS concentration in treated gas (ppmv)	9.7	3.3
H_2S concentration in treated gas (ppmv)	<1.0	<1.0
Mercaptan concentration in treated gas (ppmv)	<1.0	<1.0
Solvent flowrate, USgal/min (m^3/hr)	986 (224)	1350 (307)
LRHX duty, MMBtu/hr (Gcal/hr)	51.8 (13.1)	31.0 (7.80)
Lean cooler duty, MMBtu/hr (Gcal/hr)	−16.2 (−4.08)	−37.7 (−9.50)
Condenser duty, MMBtu/hr (Gcal/hr)	−8.98 (−2.26)	−15.8 (−3.97)
Reboiler duty, MMBtu/hr (Gcal/hr)	20.1 (5.07)	57.3 (14.4)
Absorber diameter, ft (m)	6.98 (2.13)	7.69 (2.34)
Regenerator diameter, ft (m)	5.24 (1.60)	7.96 (2.43)
Methane recovery (%)	96.6	99.3
Ethane recovery (%)	88.9	98.0
Propane recovery (%)	80.2	97.8
Butane recovery (%)	54.2	97.2
Pentane recovery (%)	19.4	95.0
Hexane recovery (%)	0.84	91.4

Case 3: High Acid Gas

Due to the high acid gas content present in this case, any gas treating solution must be designed with a high liquid-to-gas (L/G) ratio. In this case, the comparison focuses on the amine-based and hybrid solvents both cooled to 120°F (48.9°C). While the hybrid solvent outperforms the amine-based solvents in terms of mercaptan removal efficiency, the high L/G ratio enables the amine-based solvents to still meet the total sulfur specifications.

The performance results for this case are summarized in **Table 6**. High acid gas levels allow both solvents to achieve high-rich loadings. To meet the target of 10 ppmv total sulfur in treated gas, the hybrid solvent requires 2% less circulation than the amine-based solvent. The hybrid solvent also uses 14% less reboiler duty for regeneration, most of which is due to its lower water content and its enhanced regeneration efficiency.

Tower diameters are comparable between the two solvents. However, the amine-based solvent demonstrates superior hydrocarbon recovery, whereas the hybrid suffers from hydrocarbon losses due to its physical solvent component and elevated flowrate. For scenarios involving high acid gas concentrations and moderate levels of mercaptan and COS, the final design will be determined by hydrocarbon recovery requirements and operating costs.

Table 6 – Simulation Results Using Aqueous Amine-Based and Hybrid Solvents for Case 3

Parameter	**Amine-Based Solvent**	**Hybrid Solvent**
CO_2 concentration in treated gas (ppmv)	<1.0	<1.0
COS concentration in treated gas (ppmv)	1.1	<1.0
H_2S concentration in treated gas (ppmv)	3.4	<1.0
Mercaptan concentration in treated gas (ppmv)	4.6	<1.0
Solvent flowrate, USgal/min (m^3/hr)	1996 (453.3)	1953(444)
LRHX duty, MMBtu/hr (Gcal/hr)	41.6 (10.5)	33.0 (8.32)
Lean cooler duty, MMBtu/hr (Gcal/hr)	−75.9 (−19.1)	−70.0 (−17.7)
Condenser duty, MMBtu/hr (Gcal/hr)	−27.9 (−7.03)	−18.6 (−4.68)
Reboiler duty, MMBtu/hr (Gcal/hr)	109 (27.4)	94.0 (23.7)
Absorber diameter, ft (m)	8.05 (2.45)	8.14 (2.48)
Regenerator diameter, ft (m)	10.6 (3.22)	10.0 (3.05)
Methane recovery (%)	99.4	98.9
Ethane recovery (%)	99.3	97.8
Propane recovery (%)	99.5	97.8
Butane recovery (%)	99.5	96.5
Pentane recovery (%)	99.4	92.7
Hexane recovery (%)	99.3	80.8

Case 4: Molecular Sieve Regeneration Gas

Molecular sieve regeneration gas often contains elevated concentrations of sulfur components, particularly mercaptans, which are desorbed during the heating cycle used to regenerate the adsorbent beds. These sulfur-rich off-gases pose challenges for downstream processing and environmental compliance. Solvent technologies, especially physical solvents, are commonly employed to treat this stream due to their high solubility for organic sulfur species and ability to operate under high-pressure conditions. Their effectiveness in removing mercaptans from regeneration gas helps to ensure product quality and to reduce sulfur emissions, making them a critical component in integrated gas treating systems. The feed gas is at a flowrate of 100 MMSCFD, a pressure of 950 psig (65.5 barg) and temperature of 77°F(25°C). In this case the physical solvent is cooled to 40°F (4.4°C) through refrigeration while the hybrid solvent is air cooled to 120°F (48.9°C). Performances of hybrid and physical solvents were evaluated and compared in **Table 7**.

Table 7 – Simulation Results Using Hybrid and Physical Solvents to Design for Case 4

Parameter	**Physical Solvent**	**Hybrid Solvent**
H_2S concentration in treated gas (ppmv)	<1.0	1.7
Methyl Mercaptan concentration in treated gas (ppmv)	8.7	7.6
Solvent flowrate, USgal/min (m^3/hr)	381 (86.6)	719 (163)
LRHX duty, MMBtu/hr (Gcal/hr)	21.1 (5.31)	26.3 (6.64)
Lean cooler duty, MMBtu/hr (Gcal/hr)	−6.54 (−1.65)	−14.6 (−3.69)
Condenser duty, MMBtu/hr (Gcal/hr)	−2.06 (−0.518)	−8.47 (−2.13)
Reboiler duty, MMBtu/hr (Gcal/hr)	5.99 (1.51)	27.9 (7.04)
Absorber diameter, ft (m)	5.28 (1.61)	5.89 (1.80)
Regenerator diameter, ft (m)	2.97 (0.906)	5.32 (1.62)
Methane recovery (%)	98.9	99.3
Ethane recovery (%)	96.2	97.1
Propane recovery (%)	93.3	95.6
Butane recovery (%)	84.1	94.4
Pentane recovery (%)	71.5	90.8
Hexane recovery (%)	49.4	87.5

The physical solvent requires lower solvent flow compared to the hybrid solvent (381 vs. 719 USgal/min). This is primarily due to the physical solvent's strong affinity for mercaptans shown in **Table 3**, which enhances removal efficiency without excessive circulation. This lower flow rate, combined with reduced steam demand for regeneration, results in a smaller regenerator diameter and consequently lower capital and operating costs. Energy duties further reinforce this advantage: the physical solvent's required reboiler duty is 5.99 MMBtu/hr, whereas the hybrid system requires 27.9 MMBtu/hr. Similarly, lean cooler and condenser duties are substantially lower for the physical solvent, highlighting its efficiency in both energy consumption and equipment sizing. Overall, the physical solvent offers a more cost-effective and energy-efficient solution for mercaptan removal from regeneration gas. In such applications, mercaptan removal is the limiting factor while CO_2 slip is desirable.

Case 5: Trace Sulfur

Table 8 presents a comparison between the physical and hybrid solvents. While there is no specific CO_2 removal requirement for the treated gas, the physical solvent allows most of the incoming CO_2 to slip through, whereas the hybrid solvent captures most of it. Both solvents perform similarly in terms of H_2S removal. However, the hybrid solvent shows enhanced performance in removing COS, while the physical solvent is more effective in eliminating mercaptans. It is worth emphasizing that the physical solvent is cooled to 40°F (4.4°C) through refrigeration while the hybrid solvent is only air cooled to 120°F (48.9°C).

From a process design standpoint, the physical solvent system necessitates approximately double the solvent circulation rate relative to the hybrid solvent, resulting in increased thermal duties across heat exchangers due to elevated flow rates. Nevertheless, the physical solvent demonstrates moderately lower reboiler duty, attributable to its superior regeneration efficiency.

Finally, when it comes to hydrocarbon recovery, the hybrid solvent significantly outperforms the physical solvent. Overall, the hybrid solvent is a more effective choice for this application.

Table 8 – Simulation Results Using Hybrid and Physical Solvents to Design for Case 5

Parameter	Physical Solvent	Hybrid Solvent
CO_2 concentration in treated gas (ppmv)	8500	<1.0
COS concentration in treated gas (ppmv)	9.4	2.1
H_2S concentration in treated gas (ppmv)	<1.0	<1.0
Mercaptan concentration in treated gas (ppmv)	<1.0	7.8
Solvent flowrate, USgal/min (m^3/hr)	657 (149)	329 (74.6)
LRHX duty, MMBtu/hr (Gcal/hr)	33.9 (8.55)	11.6 (2.93)
Lean cooler duty, MMBtu/hr (Gcal/hr)	−10.7 (−2.71)	−5.07 (−1.28)
Condenser duty, MMBtu/hr (Gcal/hr)	−5.64 (−1.42)	−4.25 (−1.07)
Reboiler duty, MMBtu/hr (Gcal/hr)	9.62 (2.42)	13.0 (3.27)
Absorber diameter, ft (m)	6.20 (1.89)	5.91 (1.80)
Regenerator diameter, ft (m)	3.93 (1.20)	3.83 (1.17)
Methane recovery (%)	98.1	99.8
Ethane recovery (%)	93.7	99.3
Propane recovery (%)	88.8	98.9
Butane recovery (%)	73.6	98.2
Pentane recovery (%)	51.3	97.1
Hexane recovery (%)	16.7	94.4

An alternative to case 5 is one where COS is not present in the feed gas. Case 5 was rerun without COS, and the corresponding updated results are shown in **Table 9**. Key observations include a slight reduction in the hybrid solvent circulation rate, as total sulfur remains constrained by the presence of mercaptans in the feed gas. The elimination of COS led to a significant decrease in the physical solvent circulation rate, and the total sulfur becomes constrained by H_2S. Overall, the physical solvent flowrate remains considerably higher than that of the hybrid. Despite the additional flow, the physical solvent requires less reboiler duty to regenerate the solvent. Additionally, the physical solvent's hydrocarbon recovery showed moderate improvement, primarily due to the lower solvent flowrate. Overall, the hybrid solvent remains the more favorable solvent for this case.

Table 9 – Simulation Results Using Hybrid and Physical Solvents to Design for Case 5 Alternate

Parameter	Physical Solvent	Hybrid Solvent
CO_2 concentration in treated gas (ppmv)	8900	<1.0
H_2S concentration in treated gas (ppmv)	9.6	<1.0
Mercaptan concentration in treated gas (ppmv)	<1.0	9.4
Solvent flowrate, USgal/min (m^3/hr)	492 (112)	319 (72.4)
LRHX duty, MMBtu/hr (Gcal/hr)	24.8 (6.26)	11.4 (2.88)
Lean cooler duty, MMBtu/hr (Gcal/hr)	−8.55 (−2.15)	−4.79 (−1.21)
Condenser duty, MMBtu/hr (Gcal/hr)	−4.37 (−1.10)	−4.08 (−1.03)
Reboiler duty, MMBtu/hr (Gcal/hr)	7.34 (1.85)	12.6 (3.18)
Absorber diameter, ft (m)	5.90 (1.80)	5.88 (1.79)
Regenerator diameter, ft (m)	3.42 (1.04)	3.77 (1.15)
Methane recovery (%)	98.6	99.8
Ethane recovery (%)	95.5	99.3
Propane recovery (%)	92.0	98.9
Butane recovery (%)	81.9	98.3
Pentane recovery (%)	67.2	97.2
Hexane recovery (%)	41.4	94.6

Plant Data & Simulation Compatibility

Accurate modeling of acid gas removal processes is essential for optimizing solvent selection, energy efficiency, and compliance with product specifications. In this section, the predictive capabilities of our proprietary simulation tool, ProComp10, were evaluated by comparing simulated results with actual plant data. Feed gas composition of a gas plant located in the Permian Basin, Texas, currently operating on the hybrid solvent, is provided in **Table 10**. The feed gas is at a flow rate of 60 MMSCFD, pressure of 820 psig (56.5 barg), and temperature of 91°F (32.8°C). As the concentration of COS in the feed was negligible, it was excluded from the analysis. The treated gas must meet specifications of less than 4 ppm H_2S and 75% mercaptan removal (<53 ppmv of total mercaptans). The feed was evaluated with different solvents as if this were a grassroot project scenario. For comparison, separate simulations using physical and hybrid solvents were conducted, and all relevant data and results from simulations are presented in **Table 11**. The main objective here is to assess how well simulation replicates real-world performance in total sulfur removal, and the results from plant data and simulation are compared in **Table 12**. This comparison provides valuable insights regarding reliability of simulation-based design and potential troubleshooting in such applications.

In **Table 11**, physical solvent #1 presents the results for a design using non-refrigeration cooling and physical solvent #2 shows the results for the design incorporating a solvent refrigeration for cooling the lean stream.

The hybrid solvent effectively removes hydrogen sulfide and, unlike the physical solvent, allows limited hydrocarbon solubility, resulting in a greater hydrocarbon recovery. The physical solvent #1, on the other hand, is more effective in removing mercaptan but demands higher solvent flow rates and larger heat exchangers (The hybrid requires 76.4% less heat exchanger area). Lean cooler duty and regenerator reboiler duty are slightly higher in the hybrid system by 5% to 11%.

Table 10 – Plant Feed Gas Composition

Component	Value	Unit
Hydrogen Sulfide	0.92	mol%
Carbon Dioxide	1.40	mol%
Mercaptan	213	ppmv
Nitrogen	1.42	mol%
Methane	80.55	mol%
Ethane	9.31	mol%
Propane	3.95	mol%
Butane	1.63	mol%
Pentane	0.54	mol%
Hexane	0.09	mol%
Heptane	0.01	mol%
Octane	0.002	mol%
Benzene	0.03	mol%
Toluene	0.01	mol%
Argon	0.05	mol%

Table 11 – Procomp10 Results for Simulations Using Hybrid and Physical Solvents

Parameter	Hybrid Solvent	Physical Solvent #1	Physical Solvent #2
H_2S concentration in treated gas (ppmv)	<1.0	3.79	3.75
Mercaptan concentration in treated gas (ppmv)	50.3	<1.0	<1.0
Solvent flowrate, USgal/min (m^3/hr)	236 (53.6)	468 (106)	230 (52.2)
LRHX area, ft^2 (m^2)	897 (83.3)	3640 (339)	2280 (212)
LRHX duty, MMBtu/hr (Gcal/hr)	5.3 (1.3)	18 (4.5)	10.7 (2.7)
Lean cooler duty, MMBtu/hr (Gcal/hr)	−6.4 (−1.6)	−6.1 (−1.5)	−5.5 (−1.4)
Condenser duty, MMBtu/hr (Gcal/hr)	−1.7 (−0.43)	−1.9 (−0.48)	−1.4 (−0.35)
Reboiler duty, MMBtu/hr (Gcal/hr)	10 (2.5)	9.0 (2.3)	4.9 (1.2)
Methane recovery (%)	99.6	96.6	98.1
Ethane recovery (%)	99.0	89.4	93.7
Propane recovery (%)	98.7	81.1	88.7
Butane recovery (%)	98.3	60.3	74.1
Pentane recovery (%)	95.9	30.1	51.8
Hexane recovery (%)	93.8	1.9	11.5

If the lean stream in physical solvent #2 is chilled to 40°F (4.4°C), the required solvent flow can be reduced to 230 gallons per minute, which demands a chiller duty of −5.5 MMBtu/hr.

Including the amine-based solvent in the comparison revealed it required a circulation rate over three times higher than that of the hybrid solvent system, making it unsuitable for this application due to its substantially greater capital and operating costs.

Simulation data indicate that the hybrid configuration is the optimal choice for this application. Upon implementation, operational results have been satisfactory, with robust performance observed across essential treatment and recovery metrics. The simulation outcomes are consistent with actual plant data, exhibiting less than 4% deviation in all key parameters. These findings are summarized in **Table 12**, which underscores simulation's strong capability to accurately forecast required specifications. Accordingly, the ProComp10 simulation model demonstrates reliability for operational forecasting and design validation purposes.

Table 12 – Data Comparison between Plant and Simulations Using the Hybrid Solvent

Parameter	**Plant Data**	**ProComp10 Simulation**	**Error (%)**
Solvent flowrate, USgal/min	228	236	3.5
LRHX duty (MMBtu/hr)	5.1	5.3	3.9
Reboiler duty (MMBtu/hr)	9.6	10.0	4.2
Lean cooler duty (MMBtu/hr)	−6.2	−6.4	3.2

Conclusions

This study demonstrates that achieving low sulfur specifications in natural gas processing requires a nuanced approach to solvent selection, driven by feed gas composition, target product specifications, and operational constraints. Utilizing an extensive array of solvent chemistries alongside advanced simulation tools is crucial for performing tailored assessments and attaining optimal design solutions.

Simulation and plant data confirm that hybrid solvents deliver superior energy efficiency, hydrocarbon recovery, and reduced equipment sizing in scenarios where mercaptan removal requirements are moderate. Hybrid systems leverage the synergistic effects of chemical and physical absorption, enabling single-step treatment and minimizing co-absorption of hydrocarbons, which translates to lower OPEX and CAPEX for most applications.

Conversely physical solvents with high affinity for organic sulfur species prove optimal for deep mercaptan removal, especially in the absence of COS in feed gas, and for treating molecular sieve regeneration gas. This solvent exhibited high affinity towards H_2S as well. Physical solvent systems exhibit lower regenerator reboiler duty, reduced solvent circulation rates, and smaller regenerator diameters, resulting in significant operational cost savings. However, increased hydrocarbon co-absorption in physical solvent designs may necessitate additional recovery steps, impacting overall process economics beside the cost needed for refrigeration unit.

Amine-based solvents can be a viable solution for total sulfur removal in cases where the feed gas contains a large amount of H_2S. These cases require a high liquid-to-gas (L/G) ratio to remove all incoming H_2S; as a result, amine-based solvents can also remove low to moderate amounts of mercaptans.

The reliability of ProComp10 simulation tool is validated by close alignment with actual plant performance, with key process parameters; circulation rate, heat exchanger duty, and reboiler duty showing less than 4% error. This demonstrates the model's strong predictive capability for technology selection, process optimization, and operational forecasting.

Ultimately, solvent selection for acid gas removal must be tailored to the specific process envelope, balancing sulfur removal efficiency, hydrocarbon recovery, energy consumption, and capital investment. Advanced hybrid formulations and rigorous simulation enable robust, cost-effective solutions that meet evolving regulatory and product quality standards, supporting sustainable and compliant gas processing operations.

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