ENGINEERING PRACTICE

VOLUME 10 NUMBER 42

JANUARY 2024

IACPE
INTERNATIONAL ASSOCIATION OF CERTIFIED PRACTICING ENGINEERS

WWW.IACPE.COM

Can you trust your simulation software for troubleshooting?

Anand Govindarajan, Ph.D., Upasana Manimegalai Sridhar, Ph.D.
Ralph Weiland, Ph.D.

Abstract

Troubleshooting is a demanding task because, when a problem arises, a solution is usually urgently needed. Not only is the experience of the engineer essential, but also a rigorous process of root cause analysis and a reliable simulation tool are equally important to make well thought-out, sound recommendations.

This article discusses the following specifics regarding amine systems:

- How root cause analysis can be carried out
- What is data? And what is not?
- Issues with data reliability
- Data required for benchmarking

Subsequently, this article discusses some of the common issues and suggested mitigation measures in amine systems for dealing with:

- Failure to meet product quality
- Heat stable salts incursion
- Solvent loses
- Foaming
- Corrosion

For each of these issues, this article discusses the use of a simulation tool — ProTreat® — and how it is meant to be used in the context of troubleshooting, and the technically correct way to interpret the results. Finally, this work discusses a case study from an actual refinery fuel gas treating application using MDEA as the solvent. Root cause analysis principles and the benchmarking guidelines discussed here ae used as an illustrative example.

Introduction to troubleshooting

Any problem occurring during operations can cause a lower quality product or loss of production and that can represent a significant cost. The issue is even more important as oil refiners and gas producers must protect their margin. Troubleshooting is a demanding task because, when a problem arises, its solution is urgently needed; no doubt it will catch the attention of management, and the engineers will be put under a lot of pressure.

With time being of the essence, not only is the experience of the engineer essential, but also a rigorous process of root cause analysis and a reliable simulation tool are equally important to make well though-out and sound recommendations. This paper looks at troubleshooting in the context of amine systems and is meant to serve as a general guide for the use of simulation in troubleshooting.

Root Cause Analysis in Amine Systems

In engineering, root cause analysis is a series of steps used in problem solving and is a collective term that describes a wide range of techniques, tools and approaches to identify the causes of a problem. The process is well understood and goes through a few essential steps which can be generalized as follows:

- Definition of the problem
- Data collection and benchmarking
- Identification of potential root causes
- List of plausible explanations
- Testing corrective actions
- Implementation and monitoring

Table 1 provides a high-level summary based on the generalized troubleshooting steps in relation to amine systems.

Table 1: Summary of generalized troubleshooting steps

Troubleshooting step	Details
Define problem	Some typical problems associated with amine systems (illustrative, not exhaustive) • Off-spec product • Heat stable salts • Excessive solvent losses • Foaming • Corrosion
Data collection and benchmarking	• Temperature and pressure • Flow • Solvent analysis • Operating guidelines • System design limits
Identify potential root causes	Important to understand the cause effect relationships between multiple variables affecting the process and enlist all of them.
List of plausible explanations	Each root cause may have a possible explanation, and a series of steps that could explain why the problem occurs. Such explanations should be guided by data, scientific explanation, and engineering judgement. The role of experience is important, no doubt, but experience alone may not have all the answers.
Testing corrective actions	The usage of a simulation tool plays an important role in allowing testing of corrective action(s) and increases the level of confidence for the implementation of a solution. Process simulations should tell an engineer how the process is supposed to operate, given the system configuration and a set of operating parameters. Once again, far from treating process simulations as black box models, they should support deductive reasoning and not be viewed in isolation. Here, the role of experience in the utility of a simulation is important.
Implementation and monitoring	Once reasonable confidence has been established by testing corrective actions, and risks evaluated, the implementation of the proposed solution may occur. Subsequently, the unit should continue to be monitored to ensure desired objectives are met.

Data collection and benchmarking

Good detective work begins with collection of good data. Good troubleshooters do not accept data at face value, they validate the data and make decisions based upon the data, rather than speculation. When it comes to plant data, it is common to have errant data measurement as amine plants corrode or plug. Process simulators can be tuned to match some of these data. In many cases, process simulators allow arbitrary tuning of parameters in the guise of allowing flexibility to the user or allowing a photographic replication of the plant. Not only is such tuning devoid of scientific principles, in addition, if the simulation is tuned based on bad plant data it can lead to inconsistent predictions and incorrect conclusions. So, in troubleshooting validation is critical and it is a reasonable guiding principle to treat any piece of data as error prone until proven innocent. This brings us to the question - how does one ensure that plant data available on hand is good (reliable)? Some of the obvious preliminary checks include questions such as –

- Are the valves lined up to put the flow where it should go?
- Are all instruments measuring correctly?
- Are the laboratory analyses reproducible and accurate?

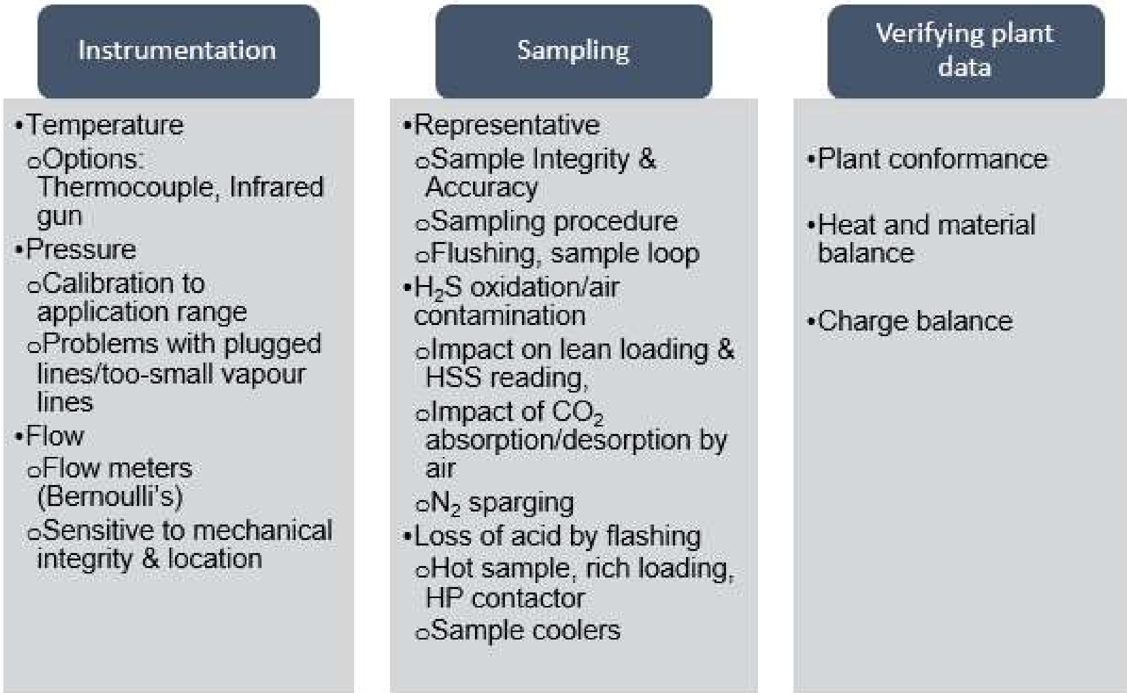

Figure 1: Troubleshooting preliminaries.

Temperature & pressure measurements

Figure 1 details some preliminary issues related to data collecting in amine systems. Starting with instrumentation – the level of trust in instrumentation is inversely proportional to instrument complexity. Collecting temperature data can be relatively simple. Options include thermocouple devices, or infrared guns. Temperature measurement devices can be miswired or improperly installed. Pressure measurements, once again simple, yet are prone to incorrect installations. Lines can be plugged, or too small diameter vapour lines can contain liquid legs trapped by joints, or incorrectly sloped vapour lines accumulating liquid. Also, it is critical to check that pressure transducers are properly calibrated to the range of pressure for the application.

Flow measurements

Measuring flow is essential, and it can be hard sometimes to diagnose malfunctions of flowmeters. The most common type of flowmeter uses an obstruction on a pipe to generate pressure difference which is then measured (based on Bernoulli's equation to infer velocity from measured pressure difference). Portable clamp-on ultrasonic flow meters are also available and at the more complex end of the spectrum, mass flow rate can be measured, even for two-phase flows. Flow meters are sensitive to mechanical integrity and solid deposit/scale can cause some problems. Their location is obviously important as you want to avoid wrong measurement if these are in a region of turbulence like downstream of a flow control device. There are other issues as well with flow meters including incorrect calculations on the DCS, corroded primary elements, defective transmitters and so on. It may sometimes be advisable to have two flow measurements and ensure they agree. In any troubleshooting exercise, correct flow measurements are essential - direct visual inspection and simple hand calculations to ensure the DCS is producing the correct output will save significant embarrassments.

Sampling

An amine sample must be representative of the amine that is circulating in the system. It is essential to follow proper sampling procedures to maintain sample integrity and accuracy. Often samples are drawn from a long sample line which may contain stagnant liquid and not be truly representative of the circulating amine. Sample integrity can be preserved by flushing the sampling line to avoid any stagnant material or better, by having a sample loop on the system and N2 blanketing. Care must be taken to avoid air ingress that can cause H2S oxidation or absorption of CO2 into the amine sample. In addition, loss of acid gas can occur by flashing as well when sample is taken from the hot section, such as the rich section or a high-pressure contactor – so it is important to cool such samples immediately by running through a cooler. More discussion on sampling is available in (Weiland, et al. 2018).

Table 2: Preliminary sanctity check requirements for plant data

Unit operation/item	Comments
Absorber	1. Does acid gas removed as calculated by gas analysis and gas flow rates agree with acid gas picked up by solvent (by solvent flow rate and loading change)? 2. Is column energy balance consistent with heat released from the heat of absorption and known inlet and outlet gas and liquid temperatures and flows? In both cases above, the material and energy balance should close within the accuracy of the basic measurements involved, if not something is wrong.
Regenerator	1. Dry acid gas flow from the overhead condenser must agree with the acid gas flow rate to the column in the rich amine minus the residual acid gas in the lean amine. 2. Is reboiler duty consistent with the measured reflux flow rate and top tray temperature? In both cases above, it is important to account the thermal state of the rich amine feed. In case there is feed flashing, it is important to understand the contribution of the flashing vapour flow to the overheads.
Charge balances (A more comprehensive discussion is available (Hatcher and Weiland 2009))	1. All solution analysis should be checked for obeying the charge balance whenever possible. Overlooking this may lead to incorrect simulations based on wrong solution analysis that do not even obey the charge balance. A charge balance spreadsheet is available free of cost at Optimized Gas Treating Inc's website https://www.ogtrt.com/free_downloads

Verifying plant data

Table 2 provides a summary of the preliminary data checks that should be carried out to ensure that the data conform to material, component, and energy balances.

Data required for benchmarking

Knowing now that our data satisfy initial sanctity tests, Table 3 is a check list that covers the physical properties, and composition of different streams. Gathering these data over multiple stable regions of operation will be useful for simulation benchmarking of the amine plant. Do note that Table 3 assumes that the hardware information related to the columns such as number of installed trays / packing height, type of the internals, column diameter, etc. are known.

Table 3: Amine system data required for benchmarking

Temperature and Pressure	▪ Feed gas ▪ Sweet gas ▪ Rich amine at bottom of absorber ▪ Lean amine at top of absorber ▪ Rich amine at the exit of L/R exchanger or control valve outlet (consistent location for T and P) ▪ Lean amine leaving reboiler ▪ Acid gas leaving the regenerator ▪ Lean amine at exit of L/R exchanger ▪ Condenser ▪ Reboiler ▪ Column overhead going into condenser ▪ Column bottoms going into reboiler
IC amine analysis	▪ Lean amine
pH	▪ Report temperatures where pH readings are taken ▪ Lean amine ▪ Rich amine
Gas flows and composition analysis	▪ Gas flows and composition analysis ▪ Feed Gas to absorbers ▪ Treated gas from absorber ▪ Acid gas leaving regenerator reflux drum
Other flows	▪ Lean amine flow ▪ Reflux flow ▪ Reboiler steam flow (also furnish T/P for thermal condition)
Acid Gas Loadings (H_2S and CO_2)	▪ Lean amine (at the outlet of lean cooler)

Common issues and suggested measures

This section attempts to layout some of the common issues and their causal factors. This is by no-means an exhaustive list. In addition, the direction of the deviation (high/low/erratic) and potential solutions are also listed in Table 4.

Expectations from simulation

Simulation tools are often trusted as a gospel without a finer understanding of the tool being used. In general, a set of input parameters are given to the simulator. The simulator then calculates how the process is supposed to

Table 4: Common Issues, causal factors, and potential solutions in amine units

Issue	Causal factor	Solution
Off-spec product (sweet gas)	Rich loading (high)	Increase circulation rate and/or amine strength
	Rich loading (maxed)	Increase amine strength
	Lean loading (high)	Check regenerator for poor stripping performance Check L/R exchanger for contamination/leaks
	Lean temperature (high/low)	Check amine cooler
	Absorber/Regenerator DP (high)	Fouled trays – cleanout maybe necessary
	Absorber/Regenerator DP (low)	Check for mechanical damages
	Absorber/Regenerator DP (erratic)	Foaming may be occurring – troubleshoot
	Regenerator temperature (low)	Increase heat to reboiler
Heat stable salt incursion (Hatcher, Miglani and Govindarajan 2020)	Contaminants from upstream processing	Some HSS precursors can be removed through water washes of inlet hydrocarbon gas (HCl and SO_2 for instance)
	Impurities in make-up water	Clean makeup water to be ensured (boiler feed water quality or better)
	Piping mis-lineups	Ensure flow is going where it is meant to
	Excessive caustic addition for neutralization	Use enough to liberate the amine to react with the acid gas. A reliable simulation should be able to tell you.
	Oxygen ingress	Blanket tanks, eliminate leaks in vacuum gas gathering equipment etc.
Solvent losses	Mechanical losses	Improve operation and maintenance practices
	Physical entrainment / vaporization	Water wash to retain the solvent. Check for foaming losses.
	Degradation	Thermal reclaiming maybe necessary
Foaming	Incursion of surface-active ingredients	Source prevention is critical as most filtration methods are ineffective
	Hydrocarbon ingress	Check the functioning of the inlet separator Purge or drain the skimmed hydrocarbon from the flash drum Controlling the lean amine temperature (typical rule of thumb is to maintain a lean amine temperature at 10 F above the feed gas, to prevent hydrocarbon condensation) Purge reflux
	Iron sulphide	Cartridge filters maybe necessary to ensure colloidal particles that increase the surface viscosity are eliminated
Corrosion	Rich loading (high)	Upper limited for carbon steel (CS) to be maintained between 0.4-0.5 mol/mol maximum (subject to other guidelines) Schedule reclaiming
	Velocity (high)	Lean amine velocity in CS: 7-10 ft/s (2.13-3.05 m/s) Rich amine velocity in CS: 3-5 ft/s (0.91-1.52 m/s) Ensure gradual changes in process conditions Manage throughput
	Additional guidelines on corrosion are available in other sources listed in the references.	

behave. A simulator may be able to solve a problem through deductive reasoning. However, it is very important to note that, the simulator cannot tell whether the piping and valves are lined up as per requirement and if the mechanical integrity is intact, the cleanliness of the amine unit and the solvent and whether the instruments are calibrated correctly and if lab test results can be trusted.

Thinking that sitting in front of a computer, working on simulations will solve all your problems, is simply not true. Simulations must be regarded as a mean to the end, not the only means to the end. Lastly, it begs reinforcing that simulations tuned to bad plant data are not better than the data themselves (Alvis, Hatcher and Weiland 2015).

About ProTreat®

The case study that follows will use ProTreat®, which is one of OGT's simulation products. OGT Simulation Software began with gas treating in 1992 and has been strictly mass and heat transfer rate-based right from the beginning. For 30 years OGT has led the way in this revolutionary modern technology and, after witnessing its power, others have followed. Today, most simulators claim some mass transfer rate-based capabilities, but only ProTreat is fully rate-based in the true meaning of the word ((OGT Inc. 2010) and allows you to simulate treating using single, multiple, and specialty amines, non-amine systems, amines mixed with a physical solvent, sour water stripping, and glycol dehydration in columns containing a vast range of trays, random packing and structured packing in absorbers, regenerators, and quench towers.

The latest gas treating addition to ProTreat simulates hybrid solvent systems in which part of a standard aqueous amine is replaced with an organic nonreactive component. Currently ProTreat can simulate up to three aqueous generic amines with sulfolane as the organic additive. Other combinations are under development. Some of ProTreat's applications and capabilities are that it can be used for acid gas removal, acid gas enrichment, tail gas treating and sour water stripping processes. Glycol dehydration, caustic mercaptan removal, LNG and ammonia can also be simulated using ProTreat. Asset integrity can be estimated using the corrosion prediction capabilities. ProTreat relates to actual hardware and tells what the plant should be doing and contains the largest commercially available database of solvents, both generic solvents and formulated solvents including INEOS, Dow and Eastman

proprietary solvents. ProTreat is a versatile tool that is flexible and integrable with downstream SRU and is a CAPE-OPEN plug.

Globally over 100 companies including the largest producers, refiners, solvent vendors, internals manufacturers, licensors, EPC, engineering, and research companies use ProTreat as their de facto simulator for gas treating.

How ProTreat® helps in troubleshooting amine systems

Issue	What ProTreat® can do
Off-spec product (sweet gas)	Affords reliable investigation of various process parameters on the performance of the amine system. ProTreat's mass transfer rate model is rich in detail and is a faithful mirror of the real world. In the language of process control, a true mass transfer rate simulation uses a distributed parameter model. Consequently, such models are mechanistic, detailed, and fully predictive. Mass transfer performance predictions have been validated against a large amount of full-scale plant performance data, and regeneration columns are simulated just as accurately as absorbers. ProTreat is 100% mass transfer rate-based and uses detailed chemistry and mass transfer calculations to predict performance of real equipment without guesswork.
Heat stable salt incursion	Use solvent analysis information to predict the impact of HSS on treatment. Also, enter estimated HSS based on guidelines to simulate impact on treatment. ProTreat contains (probably) the industry's largest database of HSS.
Solvent losses	Simulate the impact of water washes, degradation products, specify liquid carry-over in top vapour stream, vapor carry-under in bottom liquid streams
Foaming	Use the advanced features for columns to increase or decrease the interfacial area factors to understand the potential extent of foaming in the tower.
Corrosion	Setup virtual corrosion coupons to study the impact of loading, temperature, velocity, amine strength, and speciation on corrosion, for a variety of metallurgies, roughness, fittings, and sizes.

Case study

The case study deals with an amine unit that is a standard absorber-regenerator circuit of a fuel gas unit. The absorber contains 30 Nutter float valve trays with 8 ft. diameter and 62% active area. The regenerator has a diameter of 6 ft. on top and 8.5 ft at the bottom with three sections total; first section is packed with 10ft. of 2 in. metal pall rings, second section has 2 Koch flexi trays with 84% active area and the final bottom section has 18 Koch flexi trays with 8.5 ft diameter and 56.4% column active area. The feed gas flow is 38.2 MMSCFD of fuel gas at 38 C and 13.3 kg/cm2 that contains (in mol%) 39% CH_4, 14.9 % C_2H_6, 2% C_3H_8, 3.1 % C_4H_{10}, 1.2% CO_2, 16% H_2S, 10.9% H_2S and the rest being N_2, CO, and water vapor. MDEA with a strength of 42.6 wt% is being used to selectively remove the H_2S in the feed gas at 193 cum/h (850 USGPM). According to the plant, all the columns, pumps, and exchangers were at about 70-80% of their design capacity, so in essence there was no bottleneck. The treatment objective was < 4 ppmv H_2S and 16.5% CO_2 slip into the treated gas. However, the unit was currently producing around 22-25 ppmv H_2S leak and 20.5% CO_2 slip.

First, a simulation model was set up in ProTreat® based on the temperature, pressure, and flow data from the plant instruments. Amine analysis (lean) indicated the presence of degradation products and HSS, whereas the simulation used clean amines. On updating the simulation to account for the degradation and HSS, the simulation was able to nearly replicate the plant performance with 20.5% CO_2 slip and 24 ppmv H_2S leak. Importantly this was done without any arbitrary tuning – an important element in simulation benchmarking. Next the lean and rich loading of the absorber was examined and found to comply with the guidelines. Based on the mitigation measures for off-spec treating, a few actions that can be taken to re-establish satisfactory treating are – adjusting solvent circulation (step A), strength (step B), reboiler steam (step C), and lean amine temperature (step D). The following observations are then made regarding each of the possible actions in isolation:

- Step A – adjust solvent circulation - The temperature profile in figure 2 below indicates a well circulated absorber, so changing the circulation rate would not be necessary.

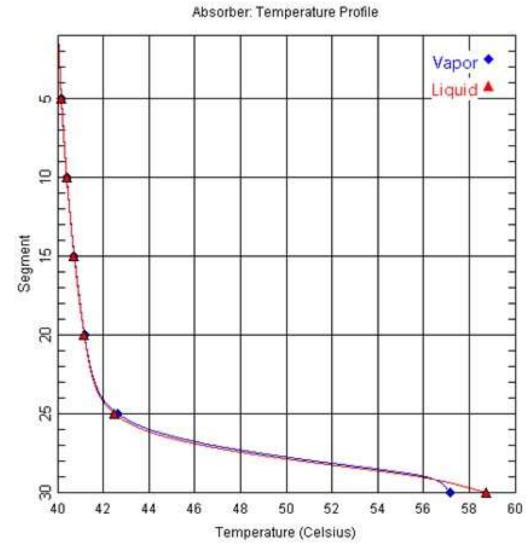

Figure 2: Temperature profile of the absorber

- **Step B** – *increase solvent strength* - The concentration profile in figure 3 clearly indicates that the absorber is lean end pinched. Therefore, increasing solvent strength will not be of use, and will worsen treating.

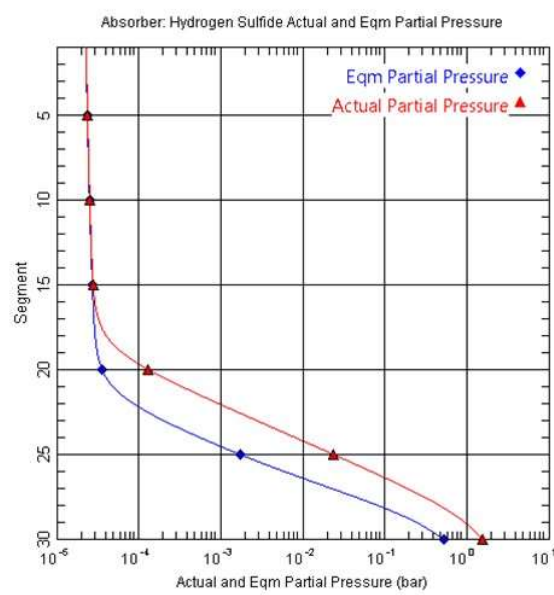

Figure 3: Actual vs equilibrium partial pressure of H_2S in the absorber

- **Step C** – *increase reboiler steam (to lower lean loading)* - Stripping the solvent to lower lean loadings than current levels may provide better treating. This is however subject to having room in the reboiler and regenerator hydraulic capacity.
  - Examining the hydraulics of the regenerator, indicated that

regenerator was at about 56 % jet flooding, and the reboiler was operating only at about 65% of capacity. This then is one of the obvious knobs to turn.

- Upon increasing the reboiler steam ratio by about 15% from 82 kg steam/m3 of solvent (0.68 lb. steam/gal) to 96 kg steam/m3 of solvent (0.8 lb. steam/gal) – the H2S leak was down to 10 ppmv and CO2 slip is around 20.3%. This was a move in the right direction with H2S, but not yet with CO2. We have not made it to the required spec yet. There was also no hydraulic limitation apparent in the regenerator on account of the increased reboiler duty. An important outcome was the lower lean loading from increasing the reboiler duty.

Step D - The lean amine temperature was about 46°C. The trim cooler would allow this to be reduced to around 40°C. Here the expectation is that the lower lean temperature will lower the H2S backpressure and allow for better treatment. Simulation indicated 17.5 ppmv H2S and 17.3 % CO2 slip. There was a stronger influence on the CO2 slip by lowering lean amine temperature than in Step C (increasing reboiler steam). H2S however was more sensitive to the Step C (increasing reboiler steam).

- Combination of Step C and Step D – resulting treating shows H2S at about 7 ppmv and CO2 slip at 17.2%

A quick comparative summary is in table 5.

Starting from about 24 ppmv H2S and 20.5% CO2 slip, the series of investigations has been able to move the plant directionally towards the desired treating of < 4 ppmv H2S and 16-17% CO2 slip. However, the plant was still not back

to the desired treating levels. One obvious option was to further increase reboiler steam, but the refinery was undertaking serious steam saving efforts, so plant personnel were not particularly keen on this. On further discussion with plant personnel, the plant mentioned that they had a mobile HSS removal skid come in and clean up and removed some HSS and degradation product a few months ago. At the face of it, this does not ring any alarm bells, however, the plant was asked to furnish a lean sample analysis before and after the HSS removal skid was brought in (see table 6 below) –

Table 5: Comparative summary of changes in KPIs

KPI	Base case	Step C (Increased reboiler steam rate)	Step D (Decreased lean amine temperature)	Step C + D together
H_2S (ppmv)	24	**10**	17.5	**7**
CO_2 slip (%)	20.5	20.3	**17.3**	**17.2**
H_2S loading in rich amine	0.46	0.453	0.454	0.452
CO_2 loading in rich amine	0.026	0.026	0.026	0.0026
H_2S loading in lean amine	0.004	**0.001**	0.004	**0.001**
CO_2 loading in lean amine	Trace	Trace	Trace	Trace

Table 6: Comparative analysis of HSS

	2 months ago	Now	
Degradation product/HSS	**Value**	**Value**	**Units**
DEA	2	0.2	wt.%
Thiocyanate	0.638	0.0447	wt.%
Formate	0.8		wt.%
Sodium ion	0.18	0.1212	wt.%
MDEA	42.7	42.61	wt.%

As observed from table 6, there was more HSS and nearly 10 times more DEA degradation product two months ago than now. The plant removed the HSS and higher degradation product due to conventional wisdom that higher amounts of these is bad for treating and corrosion.

So, at this point – the simulation run was once again updated with the HSS and degradation products from two months ago. The treated gas in the simulation produced 3.7 ppmv H2S and 16.5% CO2 slip. The lean loading is lower than the current operations (which is after cleaning out the HSS and degradation products), which might spring a surprise. HSS and degradation products have complex behaviour and there are several situations where a small quantify of HSS can benefit operations by allowing strip to leaner solvent, when the absorber is lean end pinched. The lower CO2 slip can also be attributed to the higher amounts of DEA which is a secondary amine and tends to pick up more CO2. High HSS and degradation products are not always bad, it is important to make a careful assessment with the right tools, following the right fundamental engineering principles. Given that it is not practically possible to estimate the buildup of HSS, there is no way to revert to levels of HSS that were doing the job 2 months ago. Therefore, the plant at this point was left with only option to increase reboiler steam ratio further from 96 kg steam/m3 of solvent to 108 kg steam/m3 of solvent to re-establish treating back to required levels (<4 ppmv H2S and 16.5% CO2 slip).

Conclusions

This paper was developed to be used as a general guide for using process simulation tools such as ProTreat® for troubleshooting.

- Troubleshooting can lead to consequences that are costly if not done correctly. Correctly we mean the inputs, lab analysis, constraints, and deductive reasoning from our end.
- It is always good to do a thorough root cause analysis and use a robust and versatile simulator to model and look at what is happening to the process.
- The simulator used for troubleshooting should not require adjusting arbitrary parameters to match the plant data; It should be based on mass transfer rate principles and detailed solution chemistry to be able to accurately model the process by accounting for contaminants, HSS, charge balances and solution chemistry.
- The use of ProTreat® allows troubleshooting exercises to proceed without the need to be concerned about the reliability of the simulation. Availability of reliable simulation tools with process engineering teams should not be a haggling point, they are the right way to carry out engineering.

References

Alvis, R Scott, Nathan A. Hatcher, and Ralph H. Weiland. 2015. "Expectations from Simulation." Laurence Reid Gas Conditioning Conference. Norman.

Hatcher, Nathan A., Manu S. Miglani, and Anand Govindarajan. 2020. "Design Guidelines for Heat Stable Salts Levels in Amine Systems." SulGas Conference. Mumbai.

Hatcher, Nathan, and Ralph Weiland. 2009. "Acid Gas Loading Error Analysis." Brimstone - STS Sulphur Symposium, Vail, Colorado.

OGT Inc. 2010. "Conflicted Meanings of "Rate Based"." The CONTACTOR, Vol 4, Issue 3.

Weiland, Ralph H., Nathan A. Hatcher, Clayton E. Jones, Steven M. Fulk, and Simon A. Weiland. 2018. "Accuracy of measured lean amine H2S loading." PTQ Gas.

Avoiding Environmental Cracking in Amine Units API Recommended Practice 945 fourth edition, September 2022