SIMULATION OF AMINE PLANTS: FUNDAMENTAL MODELS AND LIMITATIONS

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Synopsis

Computer simulation models are indispensable tools for designing and revamping amine plants. Accurate predictions allow engineers to properly design equipment to meet the target treating or capacity requirements, as well as operate the plant with high reliability over the life of the project.

Many simulation programs allow users to quickly and accurately design and rate equipment, to predict equipment deficiencies, and to recognize process limitations. However, not all simulation models perform equally well. This paper will review the basic fundamental theories and models that are used in amine simulation programs. We will discuss some areas of shortcomings and areas of advantages of these models and simulation approaches. Finally, we will examine some operating plant data to provide insight into how these models can be used to predict amine plant performance and the pitfalls of missing key design points.

Introduction

Performance of amine treating plants for the removal of acid gases is particularly challenging to predict, especially for industrial systems containing many components and operating over broad ranges of temperature, pressure, and concentration. To compound the complexity, amine systems also involve components that react or are absorbed at different rates in mass transfer devices that can range from structured or random packing to various types of trays.

Amines can behave in complex and counter-intuitive ways, and if unaccounted for in the design, can lead to plant operational problems, or worse, an improperly sized plant. Simplified models and computational approaches using approximation and equilibrium stage techniques are usually inaccurate, or dangerously misleading when applied to real world applications. On the other hand, an accurate model can give tremendous insight into process alternatives for improved efficiencies and optimum design.

This paper briefly discusses the foundation for simulating amine plants. Primarily, it will focus on the mass transfer rate based approach, which is the most comprehensive simulation method available today. In this approach, the gas and liquid compositions leaving the actual tray or section of packing, and the temperatures for each section of the column are precisely calculated. Examples discussed in this paper will illustrate why this is so important.

The idea to couple mass transfer with chemical reactions crystallized through the work of Astarita and co-workers. [1] These concepts were first applied to amine plants in the early 1980s. Through funding from the GAS/SPEC Technology Group of Dow Chemical (now of INEOS [note]), Weiland and co-workers [2,3] applied these approaches to develop the first mass transfer rate-based model for amine gas treating systems. Katti [4] and others within the GAS/SPEC Technology Group also took these concepts to develop a computationally fast and reliable model that later evolved into INEOS' in-house Amine Process Simulator (APS). For over 20 years, the mass transfer rate based approach has proven to be one of the most useful and reliable tools for amine plant design and modeling.

A comprehensive amine simulation model must encompass the following parts. First, the computer program must use a vapor liquid equilibrium (VLE) model based on a sound fundamental thermodynamic framework that considers accurate speciation of the chemical components. Second, the program must calculate the rate of absorption and/or desorption on real industrial trays or packing by incorporating the kinetics of reaction, the characteristics of the contacting device(s), and the effects of temperature on mass transfer. All of these variables must be considered simultaneously in order to accurately predict plant performance.

VLE Model

Vapor liquid equilibrium and chemical speciation lays the foundation for an amine simulation. The following seven equations describe the reactions that occur in a single amine, mixed acid gas system. It should be noted that Equation 7 applies only to primary and secondary amines — ternary amines such as methyldiethanolamine (MDEA) do not form the carbamate ion. Based on these reactions, twelve chemical species exist in the solution.

[note] The GAS/SPEC Technology Group was acquired by INEOS in 2001. The acquisition included exclusive ownership to all products, technology, and know-how on a global basis.

ionization of water
$2\ H_2O \Leftrightarrow H_3O^+ + OH^-$ (eq. 1)

dissociation of hydrogen sulfide
$H_2O + H_2S \Leftrightarrow H_3O^+ + HS^-$ (eq. 2)

dissociation of bisulfide
$H_2O + HS^- \Leftrightarrow H_3O^+ + S_2^-$ (eq. 3)

dissociation of carbon dioxide
$2\ H_2O + CO_2 \Leftrightarrow H_3O^+ + HCO_3^-$ (eq. 4)

dissociation of bicarbonate
$H_2O + HCO_3^- \Leftrightarrow H_3O^+ + CO_3 2^-$ (eq. 5)

dissociation of protonated alkanolamine
$H_2O + RR'R''NH^+ \Leftrightarrow H_3O^+ + R'R'R''N$ (eq. 6)

carbamate reversion to bicarbonate
$RR'NCOO^- + H_2O \Leftrightarrow RR'NH + HCO_3^-$ (eq. 7)

However, the above equations may be a simplification of the solution chemistry because amine solutions are rarely clean in industrial applications. Contaminants such as heat stable salts and amine degradation products can greatly increase the complexity of the chemistry. Intentionally added chemicals such as caustic to neutralize the heat stable salts, or another amine introduced during a running solvent conversion, can also confound the VLE. These chemicals introduce ionic species that shift the equilibrium reactions and the solubility of acid gases. In these cases, a model that can accurately predict the effects of all components in the solution is preferred. Ultimately, an experienced amine supplier with knowledge of similar systems can provide valuable recommendations on the correct design or operating criteria to account for the effects.

The Kent-Eisenburg [5] model was one of the early methods used for estimating amine solution VLE. This model is included as an option in some commercial simulation packages. The advantage of this model is that it is computationally simple. However, it lacks the predictive capabilities of other models because it assumes ideal behavior in both the vapor and liquid phase. The parameters for the model were obtained by varying the equilibrium constants for the above equations 1 to 7 to match experimental data. Since MDEA does not form a carbamate, the model loses a degree of freedom with one less adjustable parameter. Therefore, this model should not be extended to regions outside of the experimental data. Also, this model should not be applied to systems containing MDEA or multiple amines.

Other VLE models have been developed by researchers to improve the predictions of the chemical species. For example, the Deshmukh and Mather model [4] and the electrolyte NRTL [7,8,9,10,11] model have both been used successfully to rigorously represent amine systems. Both use activity coefficients to account for the solution chemistry and therefore can be used to predict ionic and molecular species that are important in the development of rate-based models. Since these models use fundamental approaches, the models can be extended to mixed acid gas, mixed amines systems, and more recently, amine systems with heat stable salts.

The GAS/SPEC Technology Group of INEOS has been using forms of the Deshmukh-Mather and the e-NRTL in their in-house amine modeling tools for the past 20 years. Weiland successfully extended the Deshmuhk-Mather model for handling complex amine systems with heat stable amine salts in the ProTreat™ simulation program. Other more recent VLE correlations include the Li-Mather model.

There are also many "all-purpose" simulation tools that contain models that are applicable for a host of chemical processes. As these simulation models are not specialized for amine systems, the models may not be rigorously tested or updated. Users should use caution when applying these models because some models may require additional information such as equilibrium constants and interaction parameters for the system of interest. In some cases, parameters must be regressed from raw VLE data beforehand. Finally, many basic all-purpose simulators lacked the mass transfer and reaction rate algorithms to simulate an amine plant accurately.

Chemical Kinetics and Mass Transfer

In addition to VLE, a comprehensive model must also consider the reaction rates of the components. Hydrogen sulfide (H_2S) reacts with the amine via proton transfer reactions producing sulfide and bisulfide ions. These reactions are instantaneous. The reactions of carbon dioxide (CO_2), however, proceed at a finite rate. For example, CO_2 reacts with a tertiary amine such as MDEA at a relatively slow rate. This difference in reaction rates allows MDEA to be much more selective for absorbing H_2S than CO_2.

In additional to the chemical reaction kinetics, mass transfer rates must be calculated by the simulation. Mass transfer rates are determined by the tray count, the tray type, weir height, and number of flow paths. In the case of packing, mass transfer rates are calculated from the depth, type, size, and material of the packing.

Mass transfer rate is the product of the mass transfer coefficient, the interfacial area, and the concentration driving force. Gas and liquid side mass transfer coefficients and interfacial areas are usually correlated for equipment for non-reactive processes. The effect of chemical reaction is taken into account separately in the form of an enhancement factor. The enhancement factor may be calculated from kinetics information and from a diffusion model (film model, surface renewal, etc.) as shown in equation 8.

$$N_i = E_i \, k^\circ_{i,L} \, a \, (y_i^{\text{interface}} - y_i^{\text{Bulk}}) \qquad \text{(eq 8)}$$

N_I = transfer rate
E_i = enhancement factor
$k^\circ_{i,L}$ = Mass transfer coefficient
a = interfacial area
$y_i^{\text{interface}}$ = acid gas conc. at interface (from Henry's law)
y_i^{bulk} = acid gas conc. in bulk (from VLE)

It is important to note that mass transfer, chemical kinetics, and heat transfer rates are all inter-dependent. Temperature affects the reaction rates and the equilibrium behavior of the amine

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system that in turns affects the mass transfer rates. Conversely, the mass transfer rate affects the reaction rates and the amount of heat released in the absorber.

Mass Transfer Rate Approach versus Equilibrium Approach

Many computer models use an equilibrium stage approach or a simplified rate approach to simulate amine plants. The equilibrium stage approach uses the concept of tray efficiencies to correct for the differences between equilibrium stage and actual tray performance. Efficiency factors are used to estimate the variables of contact time (gas/liquid rates and weir heights), interfacial area (tray bubbling area and tray type), and acid gas driving forces. Actual efficiency varies from tower to tower, even from tray to tray. Therefore, equilibrium approach methods can lead to errors in performance prediction. The efficiency factors do not account for the inter-dependence between vapor liquid equilibrium, mass transfer, and reaction rates.

By the same token, simulation models that use simplified rate approaches can also provide misleading results. Although many models do consider the reaction rates of the amine with acid gases, they still rely on empirical tray efficiencies or tray correlations. These programs will typically translate tray or packing information back to equilibrium stages. For example, these programs may assume 3 to 4 trays per stage throughout the column, regardless of composition, temperature, flows, and other process conditions.

For a mass transfer rate based model, there is no guessing the number of trays or height of packing needed for a particular application. The mass transfer characteristics of the contacting device must be entered into the program before calculations can proceed. Therefore, the input requires detailed information about the tray or packing of interest. The composition and temperature at every point of the column is predicted. This type of model provides us with the most accurate information for plant design and optimization.

The remainder of this paper examines how a rate based simulation model can be used to predict amine plant performance and improve plant operations. The paper will point out some key design areas that sometimes are missed in other types of models. ProTreat was selected as the software for simulation of these cases as it is the only commercially available mass transfer rate based software that has the capabilities to accurately model the MDEA systems, GAS/SPEC Specialty Amines, and heat stable salts used in the following case studies.

Case Study 1

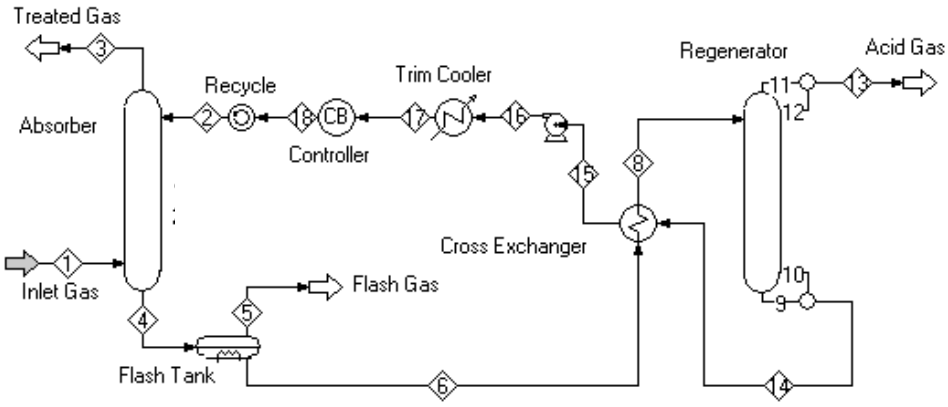
Simulation of the current plant conditions is an important step in determining whether the plant is performing to expectations. Comparisons of actual process data with a process model will often reveal areas of performance shortfalls or identify opportunities for optimization. Taken one step further, simulations can also be used to make decisions on the economics of a project or how best to utilize existing assets.

The plant in this study uses a conventional processing scheme to remove CO_2 from high-pressure coal bed methane gas. The facility was originally designed to process 279000 Nm3/h of gas containing 5 mol% CO_2. The plant meets pipeline specifications by drawing a portion of raw gas supply and processing it to a low CO_2 content. The treated gas is then blended with the remaining untreated gas to produce a 3 mol% CO_2 product gas. The amine plant was originally sized to use either DEA or a specialty solvent. However, prior to startup, the client decided to use

MDEA instead due to the lower than expected CO_2 content of the feed gas. After a year of operation, the client became concerned with the consequences of future increases in the CO_2 and, of course, wanted to maximize throughput. The inlet CO_2 content had now risen almost to the original design of 5 mol% CO_2.

To test the processing capabilities of the plant, INEOS and an engineering contractor assisted the customer in running a set of plant trials. As part of the exercise, a simulation was used to benchmark the performance data collected. A simplified PFD is shown in Figure 1.

Figure 1. PFD of High Pressure CO_2 Removal Unit



Conditions for the three tests are shown in Table 1. Test 3 was run at maximum design rates for the amine plant; Tests 1 and 2 were run at higher gas rates and in the case of test 2, at a much-reduced solvent rate. Thermocouples located on trays 3, 6 and 15 from the top of the column enabled the efficacy of the simulations to be checked not only against the overall treating performance, but also against measured tower internal temperature profiles.

Table 1. Operating Conditions for Plant Trials

	Test 1	Test 2	Test 3
Raw Gas			
Flow (Nm3/h)	235500	232100	200900
Temperature (^oC)	40	40	40
Pressure (kPa)	6881	6881	6881
CO_2 (mol%)	4.29	4.29	4.21
Lean Solvent			
Flow (m3/h)	227	186	227
Temperature (^oC)	40	43	39
Wt% MDEA	48	48	48
Acetate (ppmw)	975	975	975
Formate (ppmw)	225	225	225
Chloride (ppmw)	45	45	45

Table 2. Overall Performance Compared With ProTreat Simulation

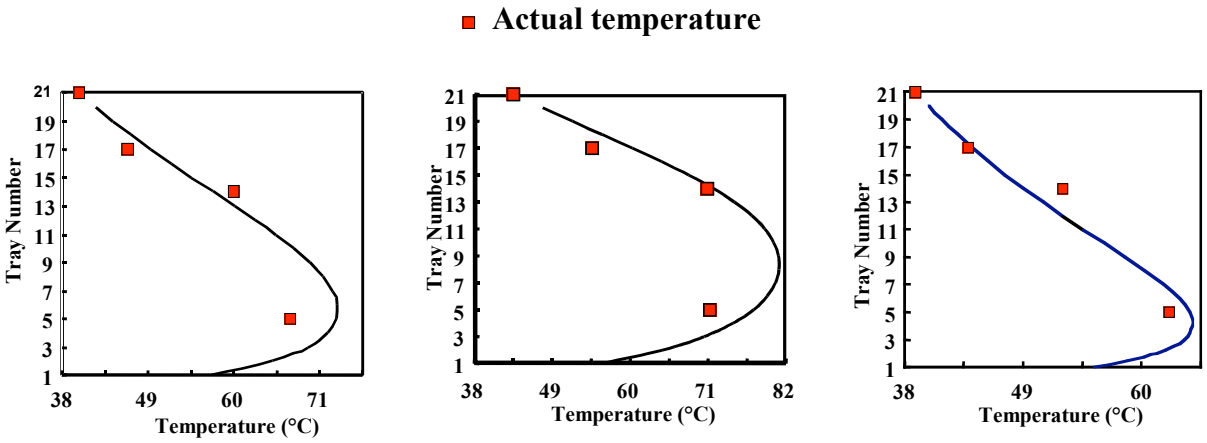
	Test 1	Test 2	Test 3
Solvent Rate (m3/h)	227	186	227
Gas Rate (Nm3/h)	235500	232100	200900
Treated Gas			
Measured CO_2 (mol%)	1.54	1.98	1.20
ProTreat CO_2 (mol%)	1.57	1.95	1.20
Lean Amine			
Measured CO_2 Loading (mol/mol)	0.008	0.008	0.007
ProTreat CO_2 Loading (mol/mol)	0.0075	0.0059	0.0046
Rich Amine			
ProTreat CO_2 Loading (mol/mol)	0.310	0.403	0.294

Simulated overall performance of both the absorber and regenerator is compared with measured test data in Table 2. Figure 2 shows temperature profiles calculated by the simulator. The points on these plots correspond to field temperature measurements. It can be seen that the level of CO_2 treat is quite accurately reproduced by the models, and even the calculated lean loads are remarkably close to laboratory measured values. In terms of temperature profiles, agreement is not perfect, but the absorber simulations fall pretty well through the middle of the data. Notice that as the circulation is reduced relative to the gas rate, the absorber temperature increases and the bulge moves up in the column. This broadening of the temperature profile coincides with increasing CO_2 level in the treated gas.

Once we had established that the model accurately simulated this system, the next step was to simulate future conditions. As indicated earlier, the CO_2 content of the gas is slowly rising. In order to understand the effect of this on treating performance, a number of simulations were performed to determine the maximum volume of gas the plant could treat at increasing increments of CO_2 concentration. For this sensitivity study, the target CO_2 level for the treated gas from the absorber was set at 2 mol% and the blended gas at 3 mol%. Figure 3 shows the effect of the inlet CO_2 content on plant capacity.

Figure 3 shows why MDEA makes economic sense when the CO_2 level is low. At CO_2 concentrations below 4.1 mol%, the plant can easily fill the downstream pipeline system with its design capacity of 502200 Nm3/h. The increasing CO_2 level can significantly reduce the capacity of the facility, and at 5.5% inlet CO_2, for example, the combined gas volume to the trunk line is cut in half.

Figure 2. Simulated Temperature Profiles Compared with Measured Data



(a) Performance Test 1 **(b) Performance Test 2** **(c) Performance Test 3**

Table 3. Operation with MDEA and GAS/SPEC CS-2010

	MDEA	CS-2010
Flow to Absorber (Nm3/h)	235500	232100
Inlet CO_2, mol%	4.29	4.5
Outlet CO_2, mol%	1.54	< 0.1
Amine Flow, Nm3/h	227	202
Maximum Total Gas Capacity (Nm3/h)	446400	502200 §

§ Currently limited by capacity of downstream pipeline

In order to address the effect of rising CO_2, INEOS proposed that the client convert the MDEA to a specialty amine called GAS/SPEC* CS-2010* Solvent. Figure 4 shows that a specialty solvent will reduce the CO_2 level in the absorber overhead to less 1000 ppmv. A specialty solvent will enable the plant to treat less gas in the absorber to a lower concentration, but maintain a higher by-passed gas flow. And indeed, about two years later, the client made the conversion to GAS/SPEC CS-2010 Solvent. Recently, at 4.5% inlet CO_2, plant personnel reported that the amine unit is processing as much as 178600 Nm3/h of gas with a higher by-pass flow. As a result of this conversion, additional gas can be by-passed and re-blended with the treated gas. This translates into an increase in the overall gas processing capacity as predicted by the model, and the change in amine has allowed the client to fully utilize their assets for maximum profitability.

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Figure 3. Maximum Capacity Using 50 wt% MDEA

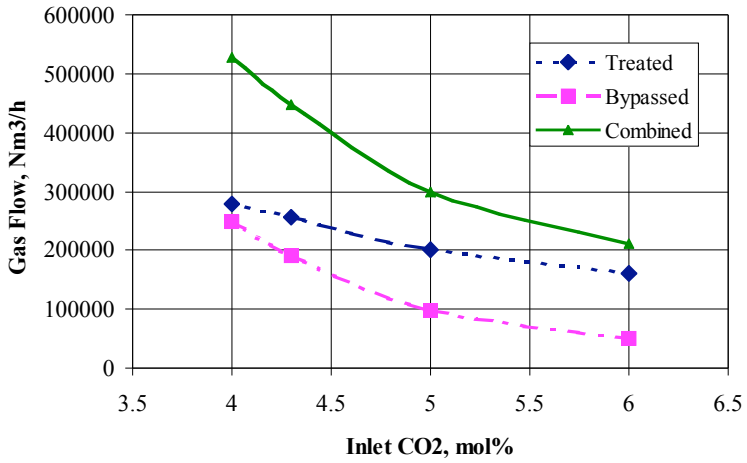
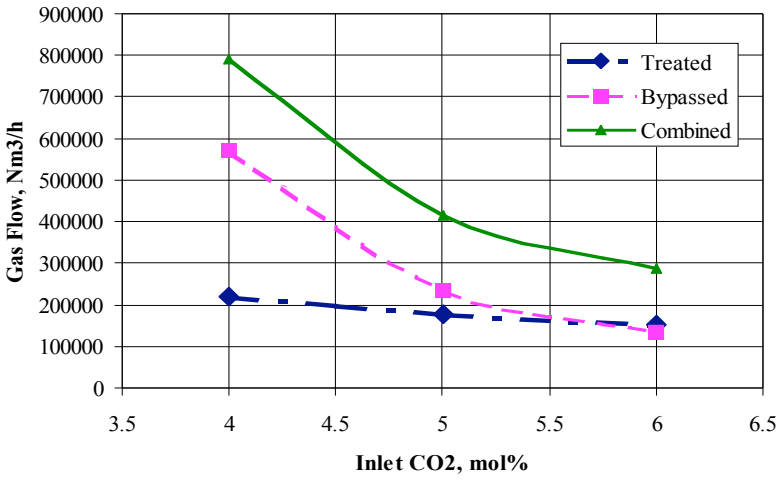


Figure 4. Maximum Capacity Using GAS/SPEC CS-2010



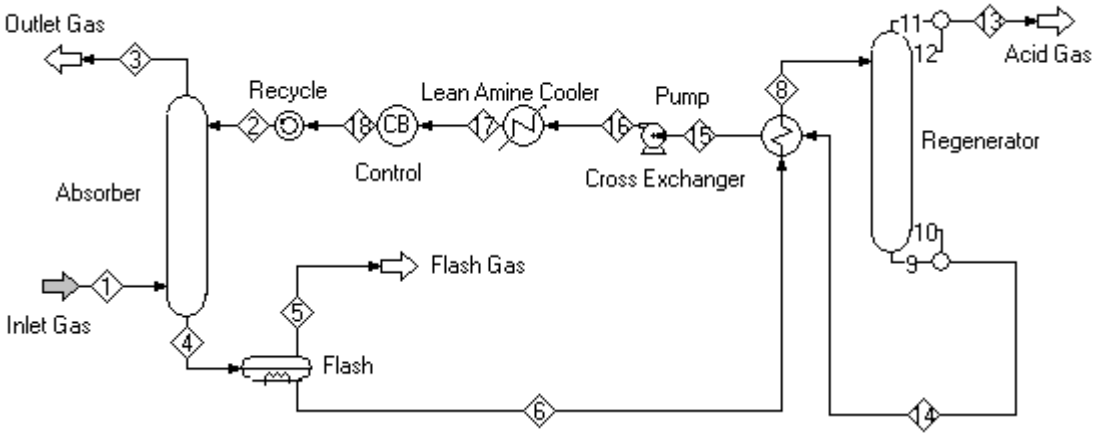
Case Study 2

The ability to predict future performance and identify process limitations can be extremely useful in natural gas applications where flows and compositions are likely to change drastically as new wells are brought into production or as treating requirements change. The following case study of an offshore application demonstrates how simulations were used to design an amine plant to accommodate expected (and somewhat unexpected) changes in process conditions. Table 4 shows the original design treating conditions. A process flow diagram is shown in Figure 5.

Table 4. Original Design Treating Conditions

Inlet Gas Flow (Nm3/h)	502200
Inlet Gas Pressure (kPa)	7419
Inlet Gas Temp (°C)	49
Gas Composition:	
CO_2 (mol%)	3.25
H_2S (mol%)	1.35
Treated Gas Specification:	
CO_2 (mol%)	< 1
H_2S (ppmv)	< 4

Figure 5. PFD of Natural Gas Plant



Early in the project, the customer and the engineering company made the key design decision to use MDEA in a plant of predetermined size. Specifically, the circulation rate, the maximum reboiler duty, and the use of a 30-tray absorber were decided before INEOS' involvement.

With the equipment parameters established, INEOS was tasked with considering the plant's performance under a range of other operating conditions. One of the main considerations was the possibility that the heat supply to the reboiler could become limited to about 57% of design at certain times. Under this, and other circumstances, the plant was to operate at the reduced rate of 279000 Nm3/h. At this stage, the engineers recognized the advantages of implementing additional feed points to the absorber to control CO_2 slip. Table 5 shows the effect of varying the feed point on treat at both design and reduced flow rates. Feed nozzles were subsequently added to trays 24 and 19 of the absorber.

Table 5. Performance at Design and Reduced Rates from ProTreat Simulation

	Design Rate	Simulation Scenario 1	Simulation Scenario 2
Gas Flow (Nm3/h)	502200	279000	279000
Feed Tray from Top	30	30	19
MDEA Conc. (wt%)	50%	50%	50%
Lean Amine (Nm3/h)	545	341	341
Treated Gas			
CO_2 (mol%)	0.92	0.59	0.99
H_2S (ppmv)	< 1 ppm	<1 ppm	< 1 ppm
Lean Loadings			
H_2S (mol/mol)	0.0002	0.0002	0.0002
CO_2 (mol/mol)	0.005	0.005	0.005
Rich Loadings			
H_2S (mol/mol)	0.13	0.11	0.11
CO_2 (mol/mol)	0.23	0.23	0.20
Reboiler Duty	X	0.57 X	0.57 X

Just before the plant started up, the customer found that a much lower CO_2 level was needed in the treated gas in order to minimize corrosion in the downstream pipeline. Therefore, instead of 1% CO_2, the plant would now have to meet a 1000 ppmv CO_2 specification. Clearly, the plant would not be able to meet this more stringent specification with generic MDEA. Since engineering and construction were already completed, the customer decided to proceed with MDEA to test the capabilities of the plant, and then eventually to upgrade to a specialty solvent to meet the 1000 ppmv CO_2 specification.

During startup, the plant experienced operational problems associated with foaming—higher than expected amounts of high-molecular-weight hydrocarbon in the feed resulted in severe foaming throughout the plant. Even with inlet gas separators and carbon filtration in place, the plant could not process more than 200880 Nm3/h and still meet the 1% CO_2 product specification. Plant personnel observed that the hydrocarbon level increased with increasing number of trays in the absorber, indicating that longer residence time in the absorber increased the condensation of heavy hydrocarbons[1]. To maintain stable operation, plant operators fed the amine to tray 19, while minimizing the amount of circulating solution. Foaming also hindered the ability to strip the MDEA solvent adequately. Table 6 shows simulations of two plant data sets. Unfortunately, the actual reboiler duties were not known, so in the simulation the reboiler duty was adjusted to give lean H_2S loadings in agreement with plant measurements.

Despite the occurrence of foaming, the simulator predicted the measured treated gas compositions with high accuracy. It should be noted that in both plant trials, the measured H_2S loading exceeded 0.002 mol/mol and the H_2S exceeded 4 ppmv in the treated gas. In order to meet specifications, the solvent would have to be stripped to a lower H_2S level than 0.002 mol/mol loading.

[1] The ProTreat simulator accurately accounts for the effect of solvent type and strength, and acid gas loadings on hydrocarbon and BTEX solubility in amine treating solutions, but does not deal with a second, liquid-hydrocarbon phase.

Table 6. Plant Trial Data Compared with ProTreat Simulations

	April	June
Inlet Gas (Nm3/h)	200880	189720
Inlet Temp (^oC)	48	35
Inlet Gas Composition		
H_2S (mol%)	2.0	2.0
CO_2 (mol%)	2.2	3.25
Solvent		
Feed Tray (from Bottom)	19	19
MDEA (wt%)	56	48
Circulation Rate (Nm3/h)	236	236
Treated Gas		
H_2S Measured (ppm)	10	5
H_2S ProTreat Simulation (ppmv)	6	7
CO_2 Measured[§] (mol%)	1.0 - 1.2	1.0 – 1.2
CO_2 ProTreat Simulation (mol%)	0.9	1.2
Lean Solvent Loadings		
H_2S Measured (mol/mol)	0.0023	0.0026
H_2S ProTreat Simulation (mol/mol)	0.0023	0.0027

[§] Plant does not have continuous outlet CO_2 measurement—Periodic basis only.

After 5 months of operation with MDEA and little or no improvement in either the foaming tendency or the CO_2 treat, it was time to implement the alternatives. The customer decided to undertake a running conversion to GAS/SPEC CS-2000 solvent. Because this solvent is much more reactive toward CO_2 than MDEA, the plant was able to meet the 1000 ppmv CO_2 specification with only 19 trays and at reduced circulation rate. An added benefit was that the higher rich loading reduced the solubility of the hydrocarbon in the amine and decreased the foaming.

Years after the conversion, the plant still runs quite well and continues to meet specifications. It is now able to treat up to 502200 Nm3/h of gas within the design circulation rate and equipment parameters.

Case Study 3

One of the key advantages of a mass transfer rate based simulator is it's ability to predict temperature profiles in the absorber. Location of temperature profile can give designers additional insight on the optimum point of operations.

In this case study, a natural gas plant looking to maximize production capacity, asked INEOS to help them determine what could be done to debottleneck the plant. Originally, the plant was designed to treat 44640 Nm3/h of gas with 7.8 mol% CO_2. Over time the CO_2 had risen to over 10 mol%. The plant run time had been very low, in the 50% range, due in part to the high CO_2 in the treated gas that caused the coldbox to freeze. The goal was to increase the maximum treating capacity by 10%, while achieving stable operations.

In order to ascertain the cause of the plant upsets, INEOS had to establish that the simulation model matched existing conditions. Table 7 summarizes the plant data and the simulated results.

Table 7. Operating Conditions for Amine Plant

	Data Set 1 (max capacity)
Flow (Nm3/h)	34600
Temperature (°C)	11
Pressure (kPa)	4440
Inlet CO_2 (mol%)	10.2
CO_2 Out (ppm)	10
ProTreat CO_2 Out (ppm)	10
Lean Solvent	
Flow (Nm3/h)	82
Temperature (°C)	48
Wt% GAS/SPEC CS-2020	50
Rich Solvent	
Temperature (°C)	79 to 81
ProTreat Temp (°C)	81

Taking this data, we first ran a simulation at 34600 Nm3/h and found the simulation matched the plant CO_2 performance at a reported CO_2 level of 10 ppm. Then, simulations were run to predict would happen at 34600, 35700, and 36800 Nm3/h at the same circulation rate. Simulations indicated the CO_2 out of the absorber increases drastically from 10 ppmv to 1552 and 4577 ppmv, respectively. The effect of increasing the gas rates is shown below in the CO_2 concentration profile in the column.

Figure 6. Column Profile - CO_2 concentration in Vapor

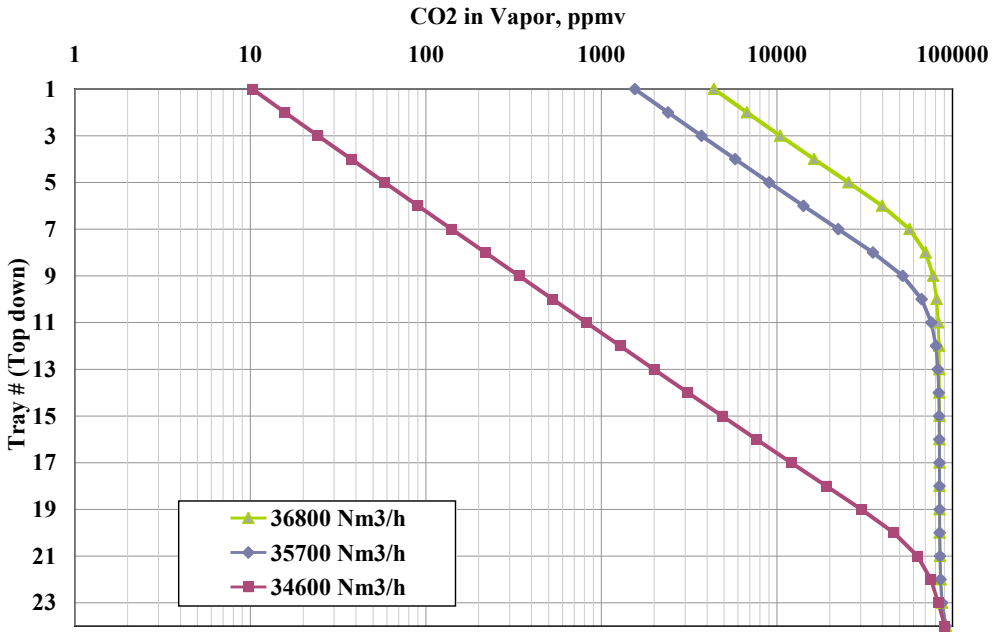


Figure 7. Column Profile – CO_2 Loadings

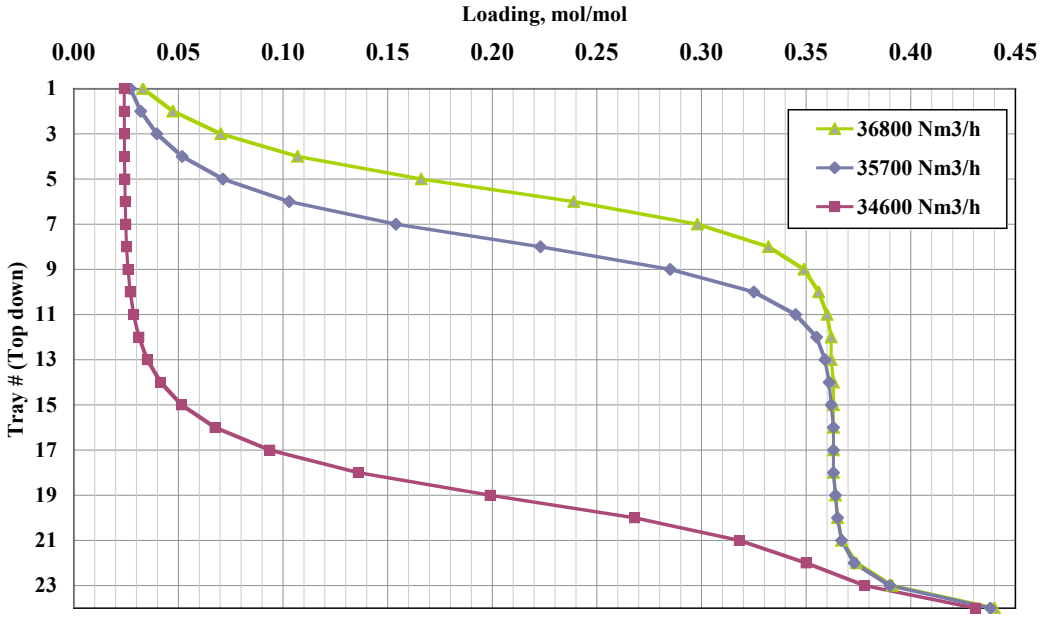
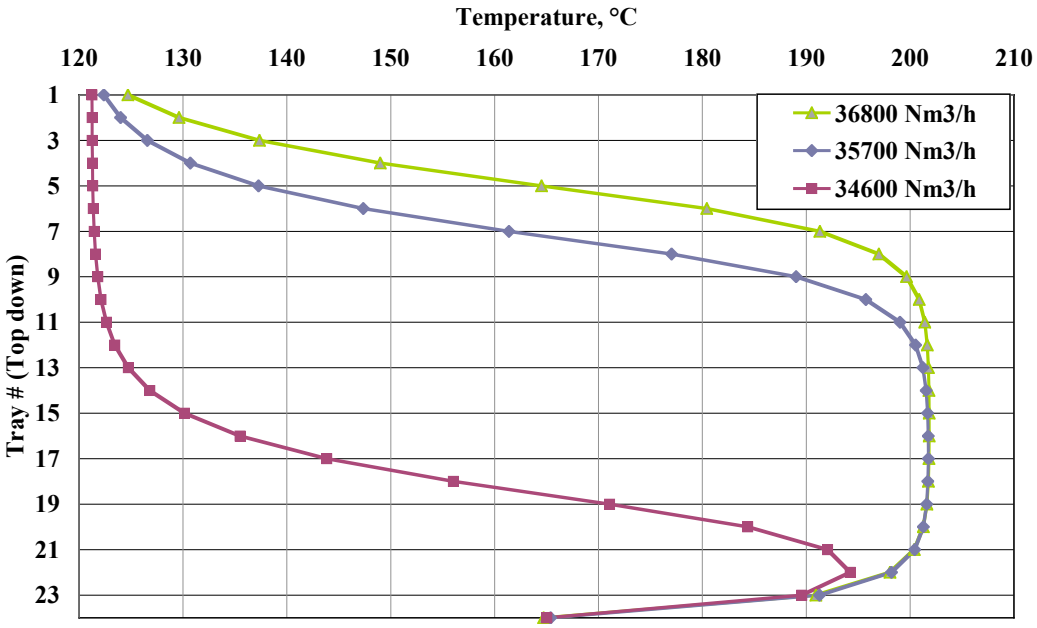


Figure 8. Column Temperature Profile.



As Figure 7 illustrates, at 35700 and 36800 Nm3/h, the CO_2 composition in the bottom 13 trays is almost constant. This indicates the amine has reached the maximum equilibrium rich loading, or is rich-end pinched, and no further CO_2 removal is possible on these trays. The other figures further illustrate why this is occurring. Figures 7 and 8 show the rich loading is at equilibrium in the bottom and middle sections of the column, correlating to where the temperature is highest.

The absorber is severely rich-end pinched as a result of the poor temperature profile. What is surprising is that as the gas flow is increased from 34600 to 35700 Nm3/h, the temperature profile undergoes a very rapid switch from showing a very high temperature bulge, to a relatively flat profile over a good part of the top section. In this transition region, plant operation would be expected to be unstable and should be avoided. And indeed, plant personnel confirmed the maximum rate of 34600 Nm3/h. They also indicated that they could only operate 15 to 30 days continuously at 32400 Nm3/h.

Many options were considered to improve the temperature profile, but it was decided that the amine circulation rate could be increased to the capacity of the pumps and exchangers. A series of simulation runs were made to determine what circulation rate would improve the treating capacity by 10%. Summary Table 8 of the simulation results indicates that the plant could treat up to 37900 Nm3/h if the pumps were upgraded to 91 Nm3/h.

As a result of this simulation study, the client is now considering an equipment upgrade to increase the capacity of the plant.

Table 8. Simulated Results of Current and Predicted Maximum Capacity

	Units	Design	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6
Inlet Gas Flowrate	Nm3/h	44640	34596	35712	36828	36828	37944	37944
Inlet CO_2	mol%	7.8	10.23	10.23	10.23	10.23	10.23	10.23
Outlet CO_2	ppmv	100	10	1552	4377	111	118	8
Circulation Rate	Nm3/h	86	81	81	81	86	89	91
GAS/SPEC CS-2020	wt%	50	50	50	50	50	50	50
Relative Reboiler Duty	% of design	1.00	0.88	0.88	0.88	0.94	0.97	0.98

Conclusions

This paper has reviewed the basic underlying theories and models for simulating amine gas treating plants. We have discussed the advantages of using a comprehensive mass transfer rate based simulator that allows us more in depth understanding of the process. Each of the case study presented points out different aspects of gas treating and how simulations can be used to understand the process, to suggest better ways of operation, diagnose a problem, or to allow more efficient operation under changing circumstances.

As shown by the examples, an existing plant using one solvent can be revamped with a new solvent and have its performance improved in several ways. Errors made in design, or decisions taken too early that prove limiting can be overcome by accurate and appropriate simulation. New gas streams and changed treating goals can be accommodated sometime by relatively simple changes, suggested by applying a highly reliable, gas treating process simulation tool.

Cirriculum Vitae

Jenny Seagraves is a Senior Research & Development Leader with INEOS GAS/SPEC Technology Group. She has 18 years of experience in the gas treating industry, primarily in amine treating. Her responsibilities include research and development, computer model development, plant design and troubleshooting. She holds a degree in chemical engineering from the University of Texas at Austin. She is a member of the American Institute of Chemical Engineers, the American Chemical Society, and the Gas Processor Association. She also serves on the advisory committee of the Laurence Reid Gas Conditioning Conference.

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