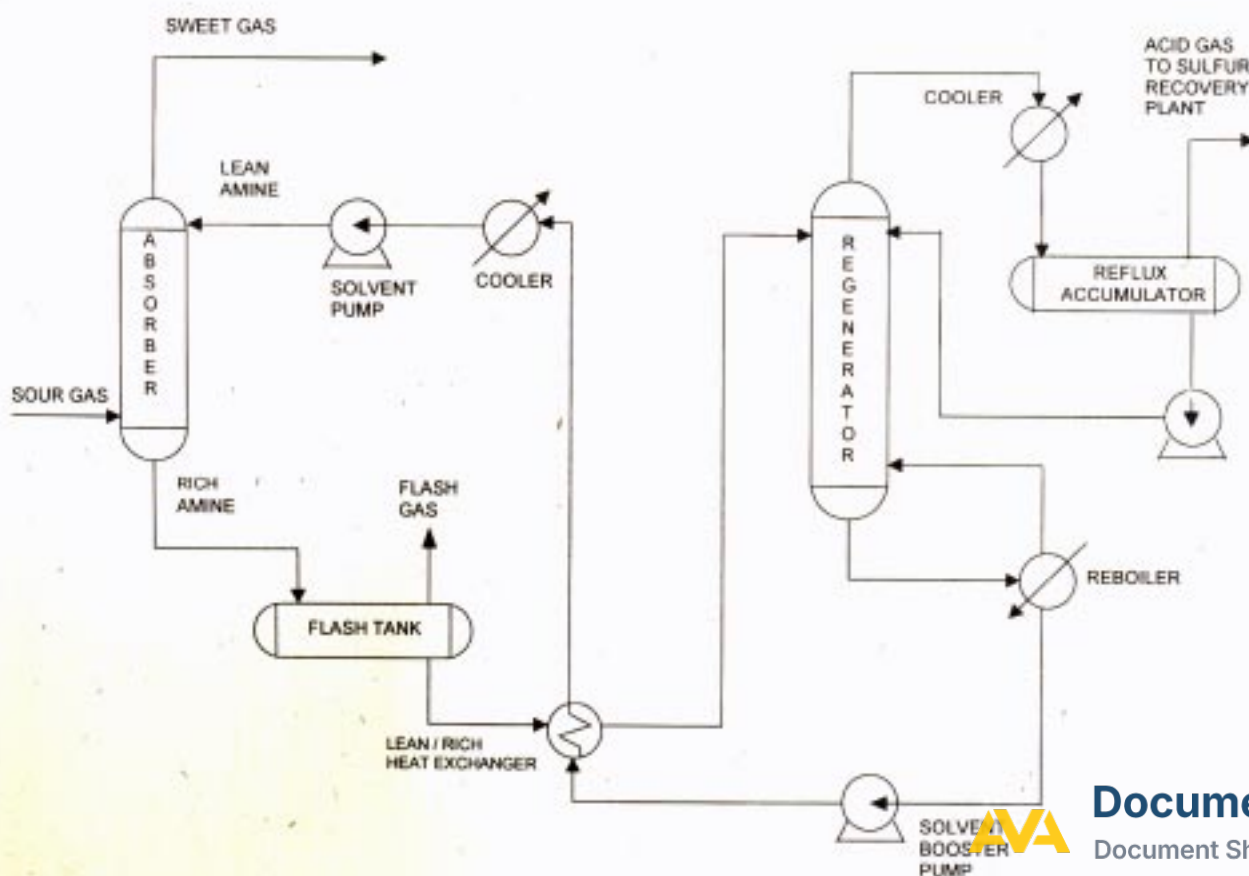


AMINE UNIT AIR EMISSIONS MODEL EVALUATION

HEALTH AND ENVIRONMENTAL SCIENCES DEPARTMENT
PUBLICATION NUMBER 4680
DECEMBER 1998



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Amine Unit Air Emissions Model Evaluation

Health and Environmental Sciences Department

API PUBLICATION NUMBER 4680

PREPARED UNDER CONTRACT BY:

DB ROBINSON RESEARCH LTD.
EDMONTON, ALBERTA CANADA

DECEMBER 1998

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EXECUTIVE SUMMARY

The implementation of the 1990 Clean Air Act Amendments (CAAA) in the United States has created the need for a reliable method to estimate and report hydrocarbon emissions from amine based sour gas and natural gas liquid (NGL) sweetening units. To address this need, a software simulation package, called Amine Unit Air Emission Model (AMINECalc Version 1.0) was developed for the American Petroleum Institute (API) by DB Robinson Research Ltd. (DBRR).

The output simulated by the AMINECalc Model is designed to suit the needs of regulatory reporting requirements. Thus, the major objective of this project is to develop a reliable and user-friendly software package that will gain acceptance by the US Environmental Protection Agency (EPA) and amine unit operators. With the intention of validating the model, API requested DBRR to evaluate the model prediction by comparing the simulation results with field data collected from operating plants. This report evaluates the model prediction as well as recommends improvements and modifications to the model to refine the predictions.

SECTION 1

INTRODUCTION

The implementation of the 1990 Clean Air Act Amendments (CAAA) in the United States has caused the need for a reliable method to estimate and report hydrocarbon emissions from amine based sour gas and natural gas liquid (NGL) sweetening units. To address this need, a software simulation package, called Amine Unit Air Emission Model (AMINECalc Version 1.0) was developed for the American Petroleum Institute (API) by DB Robinson Research Ltd. (DBRR).

Many of the amine units in the field are fitted with sulfur recovery units (SRUs) to control hydrogen sulfide (H_2S) and/or carbon dioxide (CO_2) and do not release volatile organic compounds (VOCs) and hazardous air pollutants (HAPs) to the atmosphere. However, some amine units do not have SRUs because they are used primarily to remove only CO_2 from natural gas without H_2S ; consequently some amine regenerators have the potential to release HAPs and VOCs to the atmosphere. The AMINECalc model was developed primarily for those units having the potential to emit VOCs and HAPs to the atmosphere.

The calculation algorithm of this package is based on AMSIM, a commercial software package developed by DBRR. Equipped with a rigorous non-equilibrium stage model and the Peng-Robinson equation of state, AMSIM was designed to provide accurate and reliable solutions for sour gas and liquefied petroleum gas processes. The emphasis of this commercial software package was on acid gas (H_2S and CO_2) removal, and its predictions have been constantly verified by actual plant data.

The objective of the current project is to develop a PC-based emission model to predict HAPs and VOCs from flash tanks and solvent regenerators of a natural gas sweetening unit. The AMINECalc model was re-engineered from AMSIM and enhanced to accommodate three types of calculations: mass balance calculation, gas process simulation, and NGL process simulation. The emphasis is on HAPs which include benzene, toluene, ethylbenzene and xylenes (BTEX), as well as VOCs emitted from amine units.

Amine unit operators may be required to report the emissions to the appropriate regulatory agencies. In order to gain wide acceptance by end users, special attention has been paid to the program interface design. Extensive computer literacy or simulation experience is not a requirement to operate the AMINECalc simulator. Users with a basic knowledge of WindowsTM should be at ease when using the program.

SECTION 2

THE AMINECalc MODEL

Among many treatment processes for sour gas, the absorption technology using aqueous solutions of alkanolamines is popular for economic reasons. The use of simulation software for sweetening processes has steadily increased over the years. This section will provide a general background of the amine process.

2.1 THE AMINE PROCESS

Figure 2-1 presents a process flow diagram of a typical amine-sweetening unit. The system consists of two major unit operations: absorption and regeneration. A feed stream, which is either natural gas or natural gas liquid (NGL) containing acid gases (H_2S and/or CO_2), is introduced into an absorption column where it is counter-currently contacted with an amine solution. The acid gas contents are removed through chemical reactions with the amine. After the absorbing treatment, the natural gas or the NGL is ready for consumer use or for further chemical processing.

This process is often referred to as a gas sweetening process. The treated gas or liquid is called sweetened gas or liquid while the amine solution entering and leaving the column is commonly known as the lean and rich amine solution respectively. After selectively absorbing the acid gases from the stream, the rich amine solution requires regeneration before it can be reused. The function of the regeneration column is to strip absorbed acid gases from the rich amine solution. A flash tank is commonly installed downstream from the absorber to recover dissolved and entrained hydrocarbons and to reduce the hydrocarbon contents of the acid gas product.

Together with other gaseous hydrocarbon species, hazardous air pollutants (HAPs) are potentially emitted from flash tanks and regenerators. Using the comprehensive AMINECalc model, one can estimate hydrocarbon emissions from amine sweetening units.

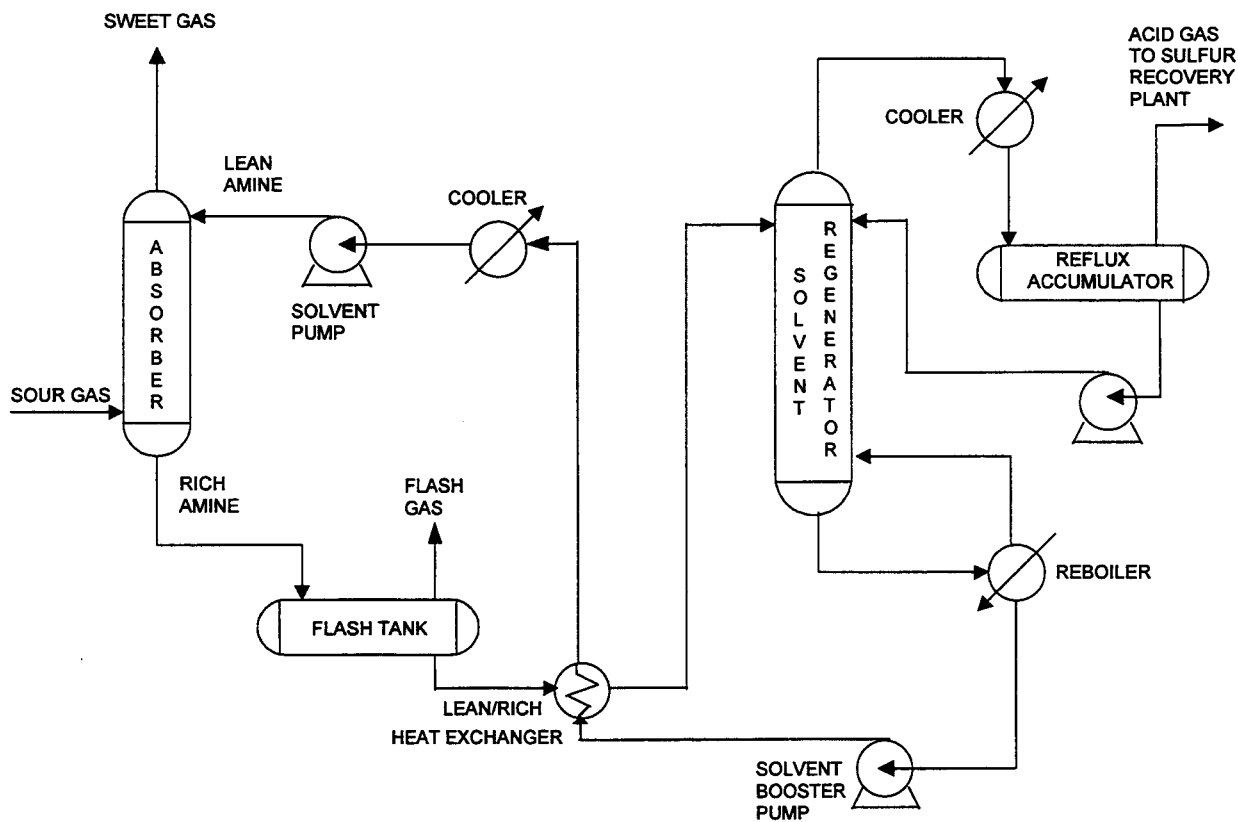


Figure 2-1: Typical Amine Sweetening Unit

2.2 MODEL DESCRIPTIONS

The AMINECalc package offers three options:

- mass balance calculation
- gas process (gas feed) simulation
- NGL (liquid feed) simulation.

The mass balance calculation option is a descriptive calculation that has the flexibility to allow users to specify their cases according to the availability of their plant data. The two simulation options allow users to perform rigorous process modeling that predicts hydrocarbon emissions from amine units based on operating conditions.

Option 1: Mass Balance Calculation

The mass balance calculation option requires input of the flow rates of lean amine stream exiting a regenerator and flow rates and compositions of the rich amine stream exiting an absorption column. As shown in Figure 2-2, a rich amine stream enters a flash tank at a pressure lower than the absorber pressure. By executing a flash calculation on the flash tank, the program calculates the flow rate and compositions of the vent gas. Simulated information of the flashed liquid and the input data of the lean amine stream are used in a mass balance calculation to give an estimate of the contents of the stripped acid gas at the top of the regenerator.

Option 2: Gas Process Simulation

The gas process simulation requires the input of sour gas feed data and lean amine circulation rate as well as the number of trays of the absorber. Figure 2-3 is the flow diagram for the sour gas treating process. The program will rigorously simulate the operation of the absorber column and calculate the hydrocarbon contents in the rich amine stream. The calculated information of the rich amine stream will then be used to predict the flows of the flash gas and the stripped acid gas of the solvent regenerator.

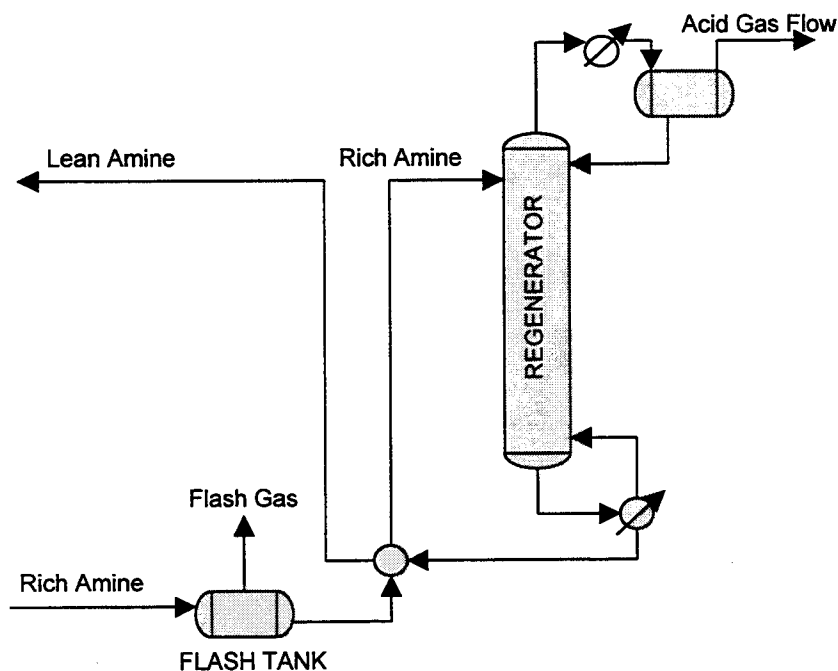


Figure 2-2 Flow Diagram for Mass Balance Calculation

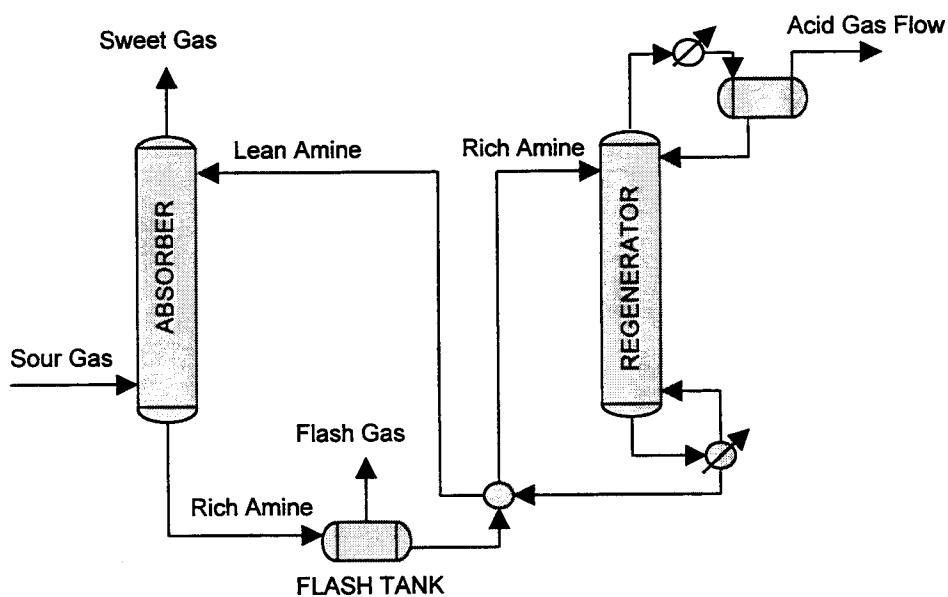


Figure 2-3 Flow Diagram for Sour Gas/NGL Process Simulation

Option 3: NGL Process Simulation

The NGL process simulation has the same flow diagram as shown in Figure 2-3 and requires the same input information. The difference between the NGL Process Simulation and the Gas Process Simulation is that the feed in the NGL Process Simulation is in liquid form and the absorber is a liquid-liquid contactor instead of a vapor-liquid absorption column. Through a liquid-liquid extraction simulation, the contents of the sweetened NGL from the top of the absorber, along with the flash vent and the regenerator vent emissions, are predicted.

2.3 MODEL INPUT REQUIREMENTS

Input requirements for each option are summarized in Table 2-1.

Table 2-1: Program Options and Input Requirements

Input Variables	Option 1 Mass Balance Calculation	Option 2 Gas Process Simulation	Option 3 NGL Process Simulation
Sour Gas Feed			
Flow rate (MMscfd)		X	
Composition (mole%)		X	
Temperature/Pressure (°F/psia)		X	
NGL Feed			
Flow rate (gpm)			X
Composition (mole%)			X
Temperature/Pressure (°F/psia)			X
Lean Amine			
Temperature/Pressure (°F/psia)	X	X	X
Flow rate (gpm)	X	X	X
Amine concentration (wt%)	X	X	X
Acid gas loading (mol acid gas/mol amine)	X	X	X
Rich Amine			
Temperature/Pressure (°F/psia)	X		
Flow rate (gpm)	X		
Composition (mole%)	X		
Absorber			
Tray numbers		X	X
Flash Tank			
Pressure (psia)	X	X	X

SECTION 3

MODEL RESULTS

This section will detail the model results and compare the predictions with actual emissions. A brief description of the model inputs and assumptions used in the model will also be presented.

3.1 MODEL INPUTS

Six sets of real process input data and emissions were used in the model simulation. First three sets of data were provided by Radian Corporation (1-3) and the other three were taken from a SPE paper (4). These data for Cases 1 and 2 were monitored and measured at sites located in Louisiana and Texas respectively. The locations of the amine unit for Cases 3 to 6 are not known.

User-defined stream characteristics and operating parameters are required to run the simulation. Summarized in Table 3-1 is the input data for the six test cases. Most of the lean solvent characteristics were taken from the actual values monitored on-site except for solvent pressure and temperature for some cases. These values were estimated using the pressure and temperature of absorber exit gas. Actual sour gas loadings for all lean solvent feeds were not available and hence were assumed.

Sour gas properties such as flow rate, pressure, and temperature that were used as model inputs were actual site-monitored values except for inlet feed gas temperature for Case 4 to 6. Detailed feed compositions for each test case can be viewed in Table 3-2.

For those unavailable operating parameters, assumptions were made or default values in the program were used. For example, a total of 20 trays were assumed for the absorber in all six test cases.

Table 3-1: Input Data for Case Simulations

Stream Characteristics	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6
<i>Lean Solvent</i>						
Type of Solvent	DEA	DEA	MEA	DEA	DEA	DEA
Solvent Weight Percent	23.0	32.0	27.2	31.8	32.4	28.5
Lean Solvent Flow Rate (gpm)	122.0	115.28	610.5	99.0	104.0	611.0
Lean Solvent Pressure (psia)	1015.0	1015.0	742.9	1025.0*	1018.0*	1008.0*
Lean Solvent Temperature (°F)	118.0	94.0	101.4	105.0*	110.0*	80.0*
H ₂ S Loading (mol/mol)	0.000	0.000	0.001	0.000	0.000	0.001
CO ₂ Loading (mol/mol)	0.001	0.010	0.010	0.010	0.0010	0.010
<i>Feed Gas</i>						
Feed Gas Flow Rate (MMscfd)	11.07	14.66	107.1	9.52	25.0	54.8
Feed Gas Pressure (psia)	1055.0	1020.0	698.7	1025.0	1023.0	1012.0
Feed Gas Temperature (°F)	84.0	94.0	86.6	105.0*	105.0*	80.0*
<i>Flash Tank</i>						
Operating Pressure (psia)	120	114	53.4	123	122	100.0

* Values were assigned due to the lack of measured data.

Table 3-2: Feed Gas Compositions in Mole Percent

Component	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6
H ₂ S	0	0	0.2*	0	0	1.0*
CO ₂	6.889	7.1495	5.5*	6.98	7.13	10.0*
N ₂	1.640	0.6824	0*	0	0.37	1.45
O ₂	0.260	0	0*	0	0	0
C ₁	81.1	83.7731	87.5*	84	84.51	82.17
C ₂	6.41	4.3549	5.3*	3.95	4.62	2.68
C ₃	1.82	1.7814	1.5*	1.75	1.74	0.55
i-C ₄	0.449	0.4614	0*	0.53*	0.412	0.16
n-C ₄	0.53	0.5536	0*	0.53*	0.459	0
i-C ₅	0.274	0.2948	0*	0.235*	0.211	0
n-C ₅	0.182	0.2030	0*	0.235*	0.137	0.058
Hexanes	0.0641	0.1400	0*	0.19*	0.153	1.0*
n-Heptane	0.0274	0.1094	0*	1.3657*	0.0055*	0.814*
Benzene	0.0350	0.0389	0.0048	0.02	0.0234	0.0275
Toluene	0.0211	0.0272	0.0012	0.0108	0.0168	0.0262
Ethylbenzene	0.0007	0.0011	0.0001	0.0006	0.0013	0.0009
Xylenes	0.0050	0.0154	0.0001	0.0029	0.0090	0.0104
C ₁₀ +	0.2382	0.2667	0*	0	0	0
n-Hexane	0.0697	0.0828	0.0289	0.2*	0.202	0.053

* Values were assigned due to the lack of measured data or reported data.

The composition of the feed gas for Case 1 and Case 2 was analyzed whereas only BTEX and n-hexane were analyzed for the feed gas in Case 3. In Case 4, feed gas compositions for C4s to C6s were not reported in the paper. As a result, based on typical sour gas compositions and known total feed gas flow rates, values were assumed for those non-measured and non-reported values such as the acid gases, C1, C2, and C3 in Case 3 as well as some other values for other cases.

Isomers of C6 alkanes (except n-C6) were grouped as “hexanes” while p, m, and o-xylenes were put together into “xylenes”. The rest of the cyclic components and non-identified HC were considered as C10+ pseudo-component.

Due to a lack of literature data of BTEX solubility in amine solutions, Henry’s constant for BTEX and n-hexane in water were employed and adjusted as temperature-independent constants in such a way that simulated emissions match with actual emissions.

3.2 RESULT COMPARISONS

The focus of this evaluation is on HAP predictions. Consequently, only BTEX and n-hexane emissions will be used as comparisons. Gas stream samplings were performed at the flash gas vent and the regenerator vent. Laboratory measurements of these samples will be summarized and compared with the model predictions. Emissions for total HAPs were computed as the sum of BTEX and n-hexane emissions. All predictions were of uncontrolled conditions. Only Cases 1, 3, and 6 reported flash emissions. These results will be compared and presented in both tabular and graphical forms for all six cases. A complete listing of the model runs can be viewed in Appendix A.

Case 1

Simulation results for Case 1 as well as the result comparison with actual emissions from solvent regenerator and flash tank can be viewed from Table 3-3 and Table 3-4 respectively.

Table 3-3: Result Comparisons for Case 1 Regenerator Vent

Species	Lab Measurement, tons/year	Simulation, tons/year
n-Hexane	0.06	0.07
Benzene	7.50	10.71
Toluene	3.50	3.35
Ethylbenzene	0.06	0.21
Xylenes	0.50	0.67
Total BTEX	11.56	14.95
Total HAPs	11.62	15.02

Table 3-4: Result Comparisons for Case 1 Flash Vent

Species	Lab Measurement, tons/year	Simulation, tons/year
n-Hexane	0.17	0.72
Benzene	0.94	2.94
Toluene	0.58	1.79
Ethylbenzene	0.02	0.08
Xylenes	0.14	0.45
Total BTEX	1.68	5.25
Total HAPs	1.85	5.98

As observed from Table 3-3, simulated emissions from the regenerator vent agree extremely well with the measured emissions except for that of ethylbenzene. Predictions within a factor of two for total BTEX and HAPs measurements are considered acceptable. On the other hand, the flash vent predictions are about three times the measured emissions as seen from Table 3-4.

Case 2

Stream samplings were not carried out at the flash gas vent for Case 2. Therefore, only regenerator vent emissions will be compared with predicted values. Measured emissions for Case 2 are controlled emissions as a BTEX stripper was used as the control measure for the amine unit. Shown in Table 3-5 are the controlled emissions that were measured on-site.

Table 3-5: Regenerator Vent Emissions for Case 2

Species	Measurement of Controlled Emissions, tons/year
n-Hexane	Neg.
Benzene	1.97
Toluene	0.85
Ethylbenzene	0.01
Xylenes	0.24

The control factor for each component is determined by the stripping efficiency of the BTEX stripper on the corresponding component. They are reported to differ for the four BTEX components (2). These values are tabulated in Table 3-6.

Table 3-6: BTEX Stripper Efficiency

Species	Stripper Efficiency, %
Benzene	70.1
Toluene	73.9
Ethylbenzene	95.6
xylenes	71.7

Because the program does not allow users to specify an individual control factor for each component to compute its controlled emission, it is necessary to calculate the potential emissions that would occur if no control measures were being employed. The uncontrolled emissions can be computed using the efficiencies of the BTEX stripper and the controlled emissions. As shown in Table 3-7, these uncontrolled emissions were summarized and compared with the program predictions.

Table 3-7: Result Comparisons for Case 2 Regenerator Vent

Species	Uncontrolled Emission, tons/year	Simulation, tons/year
n-Hexane	neg.	0.05
Benzene	6.59	9.37
Toluene	3.26	3.32
Ethylbenzene	0.23	0.26
Xylenes	0.85	1.57
Total BTEX	10.93	14.52
Total HAPs	10.93	14.57

The model predictions for Case 2 are within a factor of two of actual emissions. Predictions for total BTEX and total HAPs were a little higher than the measured emissions because benzene and xylenes were slightly over-predicted.

Case 3

The following two tables display the model predictions for Case 3 and also compare the prediction results with plant data. Predictions for n-hexane and benzene are comparable with the measured values especially for the flash vent emissions. However, others were under-predicted. For the regenerator, total BTEX and total HAPs predictions were only half the amount of actual emissions. Flash tank predictions were more agreeable with measured values if compared with the regenerator predictions.

As mentioned in section 3.1, process information especially on feed gas for Case 3 was inadequate. The majority of the simulation input was assumed instead. Thus, it is conceivable that the prediction would not meet the performance expectation.

Table 3-8: Result Comparisons for Case 3 Regenerator Vent

Species	Lab Measurement, tons/year	Simulation, tons/year
n-Hexane	0.13	0.08
Benzene	7.41	3.10
Toluene	3.41	0.66
Ethylbenzene	0.25	0.06
Xylenes	0.55	0.05
Total BTEX	11.62	3.87
Total HAPs	11.75	3.95

Table 3-9: Result Comparisons for Case 3 Flash Vent

Species	Lab Measurement, tons/year	Simulation, tons/year
n-Hexane	1.03	1.20
Benzene	1.70	1.77
Toluene	0.95	0.49
Ethylbenzene	0.13	0.04
Xylenes	0.15	0.04
Total BTEX	2.93	2.34
Total HAPs	3.96	3.54

Case 4

Only regenerator vent emissions were reported for this case. Predictions were generated for Case 4 and these results are presented in the following table. Measured flash vent emissions for this case were not available for comparisons. As observed from the following table, the simulated emissions match the field data very well. Predictions were slightly under-predicted. Predictions for both total BTEX and total HAPs are well within a factor of two of site-measured data.

Table 3-10: Result Comparisons for Case 4 Regenerator Vent

Species	Lab Measurement, tons/year	Simulation, tons/year
n-Hexane	0.16	0.18
Benzene	5.8	4.6
Toluene	2.5	1.4
Ethylbenzene	0.06	0.14
Xylenes	0.51	0.31
Total BTEX	8.87	6.41
Total HAPs	9.0	6.59

Case 5

Only regenerator vent emissions were measured for this case. As a result, there will be only one set of data for comparison. As observed from Table 3-11, most of the predicted emissions match the field data very well except for toluene. Predictions for benzene and toluene were under-predicted. Prediction for total BTEX and total HAPs is considered acceptable as these predictions are within a factor of two of measured emissions.

Table 3-11: Result Comparisons for Case 5 Regenerator Vent

Species	Lab Measurement, tons/year	Simulation, tons/year
n-Hexane	0.10	0.11
Benzene	8.2	6.1
Toluene	5.3	1.7
Ethylbenzene	0.2	0.3
Xylenes	1.5	0.8
Total BTEX	15.2	8.9
Total HAPs	15.3	9.0

Case 6

The following two tables display the result comparisons for Case 6. Predictions for the regenerator vent were reasonable except for toluene. Predictions for toluene are observed to diverge significantly from measured values in regenerator vent. As a result, total BTEX and total HAPs predictions for regenerator vent were lower than the actual emissions.

Table 3-12: Result Comparisons for Case 6 Regenerator Vent

Species	Lab Measurement, tons/year	Simulation, tons/year
n-Hexane	0.12	0.10
Benzene	42.2	41.1
Toluene	34.8	12.2
Ethylbenzene	0.94	1.38
Xylenes	10.3	3.9
Total BTEX	88.24	58.56
Total HAPs	88.36	58.66

Table 3-13: Result Comparisons for Case 6 Flash Vent

Species	Lab Measurement, tons/year	Simulation, tons/year
n-Hexane	0.47	2.35
Benzene	8.1	17.6
Toluene	7.7	13.8
Ethylbenzene	0.18	0.73
Xylenes	2.4	5.6
Total BTEX	18.38	37.71
Total HAPs	18.85	40.06

All of the species were over-predicted for the flash vent emissions. Consequently, total BTEX and total HAPs predictions were more than twice the measured emissions.