Abstract
Cumulative sour gas production of more than 6 TCF during the production history of Mozdouran reservoir from 1982 up to now, has reduced the reservoir pressure from the initial value of 6600psia to less than 5000psia at the present condition. This huge reservoir pressure drop created more than 10 degrees Celsius increase in the Khangeran refinery sour gas feed temperature (mainly due to Joule-Thompson effect) which has severe adverse effect on the performance of refinery gas treating units (GTUs). It is anticipated that the reservoir pressure reduction will continue (even more rapidly due to higher production rates and sharper decrease in gas compressibility factor) in the on coming near future. Various cooling scenarios are considered in this article to overcome the temperature rise issue. Two chemical engineering software's of HYSYS and ASPEN were recruited to investigate the effectiveness of each cooling scenario on the performance of five GTUs. The simulation results indicated that the mere sour gas cooling scenario is not sufficiently effective because of the temperature peak encountered in the contactors. On the other hand, the solvent cooling strategy was proved to be more effective from economical standpoints while leading to some technical difficulties such as heavy hydrocarbon condensations. To avoid such predicaments, both sour gas and lean solvent streams should be cooled simultaneously.

Keywords: Simulation, GTU, contactor, Joule-Thompson effect

1) Introduction
Khangeran sour gas refinery was originally founded in late 1970 decade and commissioned in early 80's. The original plant consisted of three gas treating units (GTU) refining around 30 MMSCMD Mozdouran reservoir sour gas at the peak capacity. The refinery production rate was increased to 50 MMSCMD at the beginning of new millennium by constructing two additional GTUs. All sweetening units were designed using 34% DEA solution. The amine was replaced by 45% MDEA solution, recently. The dry sour gas analysis (prepared by Amine Expert Company on 9th Feb. 2004) for the contactor feed of the Khangeran GTUs [1] were used. For all simulations, the dry gas was initially saturated with water before entering the GTU process. The average molecular weight of C_{6+} was computed about 156, based on RIPI report [1]. The sour gas contains about 10% carbon dioxide and hydrogen sulfide which should be separated using suitable amine solution in an absorption tower. The performance of amine contactor column is highly sensitive to the entering temperature of both sour gas and lean solvent. The optimal absorption temperature of H_{2}S and CO_{2} by DEA solution is about 38°C and 49°C, respectively [2]. The operational temperature for MDEA solvent is usually about 50°C [3]. Evidently, increasing the entering gas and liquid temperatures boost the maximum peak inside the absorber to a value, which is quite close to the stripping temperature of hydrogen sulfide.

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1 Di-Ethanol Amine (C_{4}H_{10}O_{2}NH)
2 Methyl Di-Ethanol Amine (C_{5}H_{13}O_{2}N)
3 GTUs number 1 and 5 were initially tested using MDEA solution in 2005. All five GTUs have been utilizing MDEA as solvent since mid 2006. It is anticipated that some GTUs will return to DEA solution again in near future due to some operational difficulties (mainly high CO_{2} concentration of the sweet gas).
Mozdouran reservoir pressure has been dropped from 6600 psia to less than 5000 psia during the past twenty
seven years (1982-2009). The reservoir gas temperature was always around 250°F (121°C). The sour gas cools
down to a temperature of 55°C (in winter) or 65°C (in summer) when entering the refinery at the pressure of
around 1070 psia. Both Joule-Thompson effect and heat transfer to the environment are responsible for this large
temperature decrease ($\Delta T = 60^\circ C$). It is shown elsewhere [1] that about 80 percent of the overall temperature
drop is due to Joule-Thompson effect for a pressure decrease of $\Delta P \approx 4000 \text{ psi}$.

The design temperature of Khangiran refinery absorption columns was considered about 52°C. To prevent
heavy hydrocarbons condensation (which leads to larger antifoam consumptions), the lean amine temperature
should be sufficiently ($\approx 2^\circ C$) higher than the entering sour gas. Evidently, increasing the feed gas
temperature from 52°C to 66°C will raise the maximum peak temperature inside the contactor (up to 95°C
which is more close to 116°C stripping temperature) and hence drastically reduces the performance of
absorption column.

Two powerful chemical engineering simulation programs (HYSYS and Aspen) were employed to simulate the
entire GTU process under the actual operating conditions, worst case (WC) when both sour gas and lean
amine enter the contactor at 70°C and also for the following cooling scenarios:

- Scenario 1 (S1): Cooling down the sour gas to 50°C while maintaining the lean solvent temperature at
  the worst case situation (70°C).
- Scenario 2 (S2): Decreasing the lean solvent temperature to 50°C while preserving the sour gas
  temperature at maximum anticipated value of 70°C.
- Scenario 3 (S3): Cooling both the sour gas and lean solvent to 50°C.

3) Simulation results for the entire GTU process

Each Khangiran refinery GTUs consists of two parallel trains with two absorbers and two strippers. The entire
refinery has five parallel GTUs with 10 contactors and 10 strippers. Although, both trains of each GTU share
the same amine and gas flash drums, however, it is always assumed that each train performs independently and there
is no interaction between two adjacent parallel contactors or strippers. Hence, the simulation results of the
simplified GTU can be easily extended to the whole sweetening process of Khangiran refinery.

The entire process of each GTU was simulated using both HYSYS and Aspen programs with the data presented
in Table 1 for the design operating variables of a typical GTU train. All five GTUs of the Khangiran refinery
sweetening processes were originally designed using 34% DEA in water as the solvent. The amine was replaced
by 45% MDEA solution, at the present condition. For this reason, all simulations were performed for both DEA
and MDEA. The computed results at various operating conditions and different cooling scenarios were compared
together.

Both HYSYS and Aspen programs have their own amine property packages. Aspen simulation software has the
additional capability of employing the so-called "Electrolyte Insert" thermodynamic package which considers
only the equilibrium model for predicting the rate of chemical reactions involved. The original Aspen "amine
package" which uses both equilibrium and kinetic models usually does not provide sufficiently accurate
predictions for MDEA solutions. For the present case study, the "amine package" was used for both HYSYS and
Aspen simulations except otherwise stated.

| Table 1: Design operating conditions of the each GTU train of Khangiran refinery |
|---|---|---|---|
| Process Variable | T(°C) | P(psia) | Rate (unit) |
| Sour gas (to contactor) | 52 | 1050 | 173000 (SCMH) |
| Lean amine (to contactor) | 53 | 1050 | 18654 $^*$ (kgmole/hr) |
| Sweet gas (form air cooler) | 38 | 1050 | 153000 (SCMH) |
| Rich amine (from contactor) | 77 | 1050 | 19400 (kgmole/hr) |
| Rich amine (from amine flash drum) | 71 | 88.9 | 19854 (kgmole/hr) |
| Acid gas (from amine flash drum) | 71 | 88.9 | 3091 (SCMH) |
| Rich amine (to heat exchanger) | 71 | 88.9 | 19854 (kgmole/hr) |
| Rich amine (from heat exchanger) | 99 | 88.9 | 19854 (kgmole/hr) |
| Lean amine (to heat exchanger) | 121 | 27.9 | 19932.8 (kgmole/hr) |
| Lean amine (from heat exchanger) | 93 | 27.9 | 19932.8 (kgmole/hr) |
| Acid gas (to air cooler) | 120 | 27.9 | 2266 (kgmole/hr) |
| Acid gas (form air cooler) | 52 | 27.9 | 2266 (kgmole/hr) |
| Stripper reflux stream | 52 | 24.7 | 1436.4 (kgmole/hr) |

$^*$ Lean amine CO$_2$ loading (0.02-0.05 mole CO$_2$/mole amine), $^*$ Lean amine flow (455 m$^3$/hr for 34 wt% DEA)
Figures 1 and 2 illustrate the predicted distributions for gas phase CO$_2$ and H$_2$S mole fractions, temperatures and gas flow rates across the entire contactor using HYSYS and Aspen software at normal operating conditions as depicted in Table 1 for various assumed Murphree efficiencies with different solvents (DEA 34% and MDEA 45% in water). The stages were numbered from the top of absorber column and stage 21 represents the entering sour gas conditions. Amine data packages were used in HYSYS simulations for both DEA and MDEA solvents and Aspen simulations of DEA solutions. This data package was not able to produce reliable predictions for MDEA simulations of Aspen program. The Electro Insert data package was imported to simulate the later case.

![Figure 1](image.png)

**Figure 1:** Temperature, gas flow rate and vapor compositions distributions for contactor using HYSYS at normal operating conditions for various efficiencies & different solvents.

Evidently, both software predict monotonic decrease in predicted gas compositions and the corresponding gas flow rates. The rate of descend increases more rapidly for larger Murphree efficiencies. The contactor stage temperatures encounter a maximum and then drop approximately to the entering solvent temperatures. This phenomenon is due to excessive rate of exothermic absorption occurring in the few bottom trays. The dilute DEA solutions react more rapidly and vigorously with both carbon dioxide and hydrogen sulfide and release lots of heats as gas enters the contactor. The more concentrated MDEA solutions react rapidly and selectively with hydrogen sulfide. Evidently, the temperature pick would be lower for 45% MDEA solution than 34% DEA solution because of less reactivity of MDEA with carbon dioxide and lower water content of the corresponding solvent. This point has been clearly demonstrated in predictions of Aspen software as depicted in Figures 1 and 2. Higher temperatures lead to larger water vapor pressures and hence higher water mole fractions in gas phase. Figures 3 and 4 demonstrate the simulation results for corresponding stripping columns with automatically computed Murphree efficiencies. For better comparison of simulation results, the HYSYS software calculated efficiencies were also used by Aspen program. Furthermore, bottom to feed ratio (or reboiler temperature) and condenser temperature were considered equal as the design specs of both simulation programs. Liquid flow rate and the corresponding CO$_2$ and H$_2$S mole fractions make more sense for stripping process. Therefore, the above parameters are plotted in Figures 3 and 4 for the entire columns. It can be seen that both simulation programs (using amine data package) produce similar reasonable results for DEA solutions. HYSYS program predicts unreasonable hydrogen sulfide composition profile across the stripping column for MDEA solution. Evidently, none of mole fractions in liquid phase can increase across the stripping tower. Aspen simulation program also performs inadequately for MDEA solution when using the amine data package. Fortunately, importing Electro-Insert (EI) data package highly improves the estimated composition profiles emphasizing large H2S selectivity of MDEA solvent.
Figure 2: Temperature, gas flow rate and vapor compositions distributions for contactor using Aspen at normal operating conditions for various efficiencies & different solvents.

Figure 3: Temperature, liquid flow rate and compositions distributions for stripper using HYSYS at normal operating conditions with different solvents.

Figure 4: Temperature, liquid flow rate and compositions distributions for stripper using Aspen at normal operating conditions with different solvents.
Figures 5 and 6 compare the predictions of HYSYS and Aspen software for worst case operating conditions (WC) with various cooling scenarios as mentioned in section one, using different solvents (DEA 34% and MDEA 45%). Again, the required Murphree efficiencies for carbon dioxide and hydrogen sulfide were automatically computed by HYSYS software. Other components efficiencies were taken as unity. For comparison purposes, the HYSYS software calculated efficiencies were also used by Aspen program.

Figure 5: Temperature, gas flow rate and vapor compositions distributions across the contactor using HYSYS program for various solvents with different cooling scenarios.

Both Aspen and HYSYS simulation programs provide quite similar predictions for temperature, gas flow rate and gas phase composition of MDEA and DEA solutions as shown in Figures 10 and 11. It should be noted that the temperature changes of both gas and liquid feeds have significant effect on absorption capacity of DEA solution. Even at worst case condition with DEA as solvent, both carbon dioxide and hydrogen sulfide concentrations are within the acceptable limits. Decreasing the sour gas feed temperature does not improve the contactor performance because of its low heat capacity. On the other hand, any temperature drop in DEA solvent stream drastically improves the absorber performance as shown in Figures 10 and 11. Since MDEA solution is very hydrogen sulfide selective, therefore its H2S absorption capacity is always extremely high and can not be affected by moderate changes in sour gas or solvent temperatures. Furthermore, such temperature changes have minor effect on the distribution of carbon dioxide concentration across the entire contactor. In all cases, the mole fraction of carbon in sweet gas stream is higher than the allowable standard values.

4) Conclusion

Mozdouran sour gas temperature has been escalated in the past two decades due to reservoir pressure drop and the corresponding Joule-Thompson effect. Various cooling scenarios have been considered in this article. The required cooling facilities were designed and the contactor absorption performance was thoroughly studied for each cooling scenario using HYSYS and Aspen simulation programs. It was clearly shown that despite of preliminary anticipations, the sour gas cooling scenario has no practical effect on the performance of contactor. The solvent cooling scenario was very effective for DEA solution but it does not affect the absorption tower performance for MDEA solution.

4 WC: Both sour gas and lean amine entering contactor at 70°C
Furthermore, the entering solvent can not be cooled below the entering sour gas temperature, because such cooling leads to excessive foaming in contactor top trays due to considerable considerations of \(\text{C}_3^+\) hydrocarbons. To achieve desirable results, both sour gas and lean solvent streams should be cooled simultaneously using previously designed air coolers.

![Graphs showing temperature, gas flow rate and vapor compositions distributions across the contactor using Aspen program for various solvents with different cooling scenarios.]

Figure 6: Temperature, gas flow rate and vapor compositions distributions across the contactor using Aspen program for various solvents with different cooling scenarios.

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6) References
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