Optimization of configurations for amine based CO$_2$ absorption using Aspen HYSYS

Lars Erik Øi$^1$*, Terje Bråthen$^1$, Christian Berg$^1$, Sven Ketil Brekne$^1$, Marius Flatin$^1$, Ronny Johnsen$^1$, Iselin Grauer Moen$^1$, Erik Thomassen$^1$

$^1$Telemark University College, N-3901 Porsgrunn, Norway

Abstract

The drawback with an absorption based CO$_2$ capture process is the large heat consumption needed for desorption. Different absorption and desorption configurations for 85% amine based CO$_2$ removal from a natural gas-based power plant have been simulated using Aspen HYSYS. A standard process, split-stream, vapour recompression and different combinations thereof have been simulated. The simulations have been used as a basis for equipment dimensioning, cost estimation and process optimization. Of the evaluated cases, a simple vapour recompression case has been calculated to be the most cost optimum configuration.

© 2013 The Authors. Published by Elsevier Ltd.
Selection and peer-review under responsibility of SINTEF Energi AS

Keywords: absorption; CO$_2$; simulation; amine; efficiency

1. Introduction

The most probable method for CO$_2$ capture from exhaust gas in the nearest future is by absorption into an amine solvent like MEA (monoethanolamine). The heat consumption for desorption is high, and there are suggested different alternative configurations like split-stream or vapour recompression to reduce this heat consumption in the literature. This paper presents simulations, cost estimation and optimization of such processes using Aspen HYSYS.

* Corresponding author. Tel.: +47-3557-5141; fax: +47-3557-5001
E-mail address: lars.oi@hit.no
1.1. Literature on alternative process configurations for \( \text{CO}_2 \) absorption

For high absorption pressures, alternative configurations have been presented in the standard reference book Kohl and Nielsen [1] and a systematic overview of alternative flow schemes for \( \text{CO}_2 \) removal from natural gas or synthesis gas at high pressures has been presented by Polasek et al. [2].

Calculations of alternative flow schemes for \( \text{CO}_2 \) removal from flue gas at atmospheric conditions have been performed by Aroonwilas and Veawab [3]. An evaluation of different stripper configurations has been presented by Oyenekan and Rochelle [4]. Recent surveys of process flowsheet modifications for energy efficient \( \text{CO}_2 \) capture from flue gas using chemical absorption have been published by Cousins et al. [5] and also Le Moullec and Kanniche [6]. Rate-based Aspen Plus simulations for such processes have been performed by Cousins et al. [7], and Fernandez et al. [8] have also performed cost estimation based on Aspen Plus simulations. Simulations with the process simulation programs Unisim and ProTreat followed by economical calculations have been performed by Karimi et al. [9].

There has been published little on calculations or simulations of alternative process configurations for \( \text{CO}_2 \) removal from flue gas, and there has been little published on economical evaluation and optimization of alternatives.

At Telemark University College Aspen HYSYS has been used to simulate a split-stream configuration and as a basis for cost comparisons by Øi and Vozniuk [10]. Øi and Shchuchenko [11] simulated different split-stream alternatives and vapour recompression alternatives in Aspen HYSYS. The simulations and results presented in this work is mainly from a Bachelor group project at Telemark University College [12].

1.2. Principles for split-stream and vapour recompression

A standard amine based \( \text{CO}_2 \) capture process has a simple absorber and a simple desorber. A traditional alternative is a split-stream configuration as in Fig 1. A partly regenerated (semi-lean) amine solution is pumped from the middle of the stripper to the middle of the absorption column, and a completely regenerated (lean) amine is sent to the top. The benefit is that the bulk \( \text{CO}_2 \) capture can be performed with only partly regenerated amine which gives lower total energy consumption for regeneration.

Fig. 1. Principle for \( \text{CO}_2 \) absorption and desorption using split-stream configuration

Fig. 2 shows the principle for the vapour recompression configuration. A regenerated amine solution from the desorber bottom is pressure reduced and led to a flash tank (lean amine flash). The liquid from the flash tank is the lean amine stream which is recirculated back to the absorber. The vapour from the flash tank is compressed and
returned to the bottom of the desorber. The vapour recompression produces a regenerated amine with less CO₂ which absorbs more CO₂ in the absorber. The temperature in the process should not exceed about 120 °C because the amine will degenerate. To avoid that, the vapour can be cooled between the flash tank and the compressor.

It is possible to combine vapour recompression and a split-stream process. This may be an improvement compared to the vapour recompression configuration because the compressor effect will be reduced. A semi-lean amine stream from the middle of the desorber can be sent to the middle of the absorption column, and the lean amine stream from the lean amine flash can be sent to the top of the absorber. A special alternative is to take the semi-lean stream from the bottom of the desorber. Fig. 3 shows such an alternative as suggested by Øi and Shchuchenko [11]. The bottom stream from the desorber is split into two streams. One part is recirculated to the middle of the absorption column (as the semi-lean stream). The other part is sent to the lean amine flash, and the liquid is recirculated to the top of the absorption column (as the lean stream).
2. Simulations

2.1. Simulation of a standard base-case process

A standard process was simulated using Aspen HYSYS version 7.2 and the simulation flowsheet is shown in Fig. 4. The calculation method is based on earlier simulations of CO₂ removal using Aspen HYSYS by Øi [13,14]. The specifications for the standard case simulation given in Table 1 is for 85 % CO₂ removal from a natural gas based power plant planned at Mongstad outside Bergen. The specifications are from the supervisor in the full scale Mongstad project from Gassnova. The amine package with the Li-Mather model [15] and non-ideal gas (using the Redlich-Kwong equation of state) was used. The Kent-Eisenberg model [16] was used for comparison. 20 stages with Murphree efficiency 0.15 and 5 K minimum temperature difference in the rich/lean heat exchanger was specified for all the simulations in this work, except for the last optimization.

Table 1. Input specifications for Aspen HYSYS standard case simulation with 85 % CO₂ removal

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet gas temperature</td>
<td>40 °C</td>
</tr>
<tr>
<td>Inlet gas pressure</td>
<td>1.1 bar</td>
</tr>
<tr>
<td>Inlet gas flow</td>
<td>108600 kmol/h</td>
</tr>
<tr>
<td>CO₂ in inlet gas</td>
<td>5.12 mol-%</td>
</tr>
<tr>
<td>Water in inlet gas</td>
<td>4.08 mol-%</td>
</tr>
<tr>
<td>Lean amine temperature</td>
<td>40 °C</td>
</tr>
<tr>
<td>Lean amine pressure</td>
<td>1.01 bar</td>
</tr>
<tr>
<td>Lean amine rate</td>
<td>129400 kmol/h</td>
</tr>
<tr>
<td>MEA content in lean amine</td>
<td>29 mass-%</td>
</tr>
<tr>
<td>CO₂ in lean amine</td>
<td>5.4 mass-%</td>
</tr>
<tr>
<td>Desorber pressure</td>
<td>2.0 bar</td>
</tr>
<tr>
<td>Heated rich amine temperature</td>
<td>105.2 °C</td>
</tr>
<tr>
<td>Number of equilibrium stages in strip</td>
<td>8(3+3+Cond+Reb)</td>
</tr>
<tr>
<td>Reflux ratio in stripper</td>
<td>0.3</td>
</tr>
<tr>
<td>Reboiler temperature</td>
<td>120 °C</td>
</tr>
</tbody>
</table>
The main result from the simulation was the heat consumption in the reboiler, which was calculated to 3.26 MJ/kg CO₂. This is a value which is lower than normally for the heat consumption in a standard CO₂ removal plant. Jordal et al. [17] give a range for different studies for 90 % CO₂ capture from NGCC plants with a value of 3.85 MJ/kg CO₂ for a standard process. Øi [13] calculated 3.65 MJ/kg for 85 % removal using Kent-Eisenberg and 3.4 MJ/kg for 82 % removal using Li-Mather. When using the Kent-Eisenberg model in this work, the calculated heat consumption was 3.39 MJ/kg CO₂. Factors like a large number of absorption and desorber stages, a low temperature difference (5K) in the amine/amine heat exchanger and a low CO₂ removal grade (85 %) can explain the low heat consumption. It is also experienced that equilibrium based calculations using Murphree efficiencies often give lower heat consumption than rate-based calculations.

2.2. Simulation of a split-stream configuration

The split-stream process in Fig. 1 was simulated in Aspen HYSYS. The specifications for the simulation were the same as in Table 1 with some changes and additions. The semi-lean feed was to stage 14. This was the optimum stage giving the lowest heat consumption. The semi-lean amine rate was 70000 kmol/h, which was close to the optimum giving the lowest heat consumption. The semi-lean CO₂-concentration was 9 wt-%. A multi-stream heat exchanger was used to simulate the heating of the rich amine stream and the cooling of the lean and semi-lean streams. In practice, this heat exchange may be performed by a system of traditional heat exchangers. The heat consumption in the reboiler was calculated to 3.25 MJ/kg CO₂ removed. This is only negligible lower than for the standard process.

2.3. Simulation of a vapour recompression configuration

The vapour recompression principle shown in Fig. 2 has been calculated in Aspen HYSYS. The Aspen HYSYS flowsheet is shown in Fig. 5. The lean amine rate achieving 85 % CO₂ removal was 115700 kmol/h and the lean CO₂-concentration was 5.2 wt-%. The vapour from the lean amine flash was cooled in a multi-stream heat exchanger so that the temperature after compression was 120 ºC. In practice, there are several ways to perform vapour cooling, e.g. by adding water. The flash pressure was 1.01 bar and the adiabatic efficiency in the compressor was 75 %. There is a potential in optimizing the process by increasing the flash pressure slightly [8].
The compressor work was multiplied with 4 and added to the reboiler heat of 2.56 MJ/kg CO$_2$ to achieve an equivalent heat consumption of 2.90 MJ/kg CO$_2$. The heat consumption is considerably lower than for a standard process. The factor of 4 for compressor work compared to heat can be explained by assuming that low pressure steam can be converted to electricity with an efficiency close to 25%. Le Moullec and Kanniche [6] and Fernandez et al. [8] use similar values of 1/0.28 and 1/0.23, respectively.

2.4. Simulation of a configuration with vapour recompression and split-stream from the bottom of the desorber

A vapour recompression process has been combined with a split-stream configuration based on a semi-lean stream from the bottom of the desorber as in Fig. 3. The number of stages in the absorber was 20 with the semi-lean feed to stage 14. The semi-lean amine rate was 50000 kmol/h and the lean amine rate was adjusted to 72900 kmol/h to achieve 85% CO$_2$ removal. The semi-lean CO$_2$ concentration was 5.6 wt-% and the lean amine concentration was 5.0 wt-%. The Aspen HYSYS flowsheet is shown in Fig. 6.

Fig. 6. Aspen HYSYS flowsheet for a configuration with vapour recompression and split-stream from the bottom of the desorber

The equivalent heat consumption in the reboiler was calculated to 3.02 MJ/kg which is not lower than for a configuration with vapour recompression. The recompression flow and compressor effect are however considerably lower than for the vapour recompression case. Several possibilities to reduce the heat consumption further were tried. The ratio of semi-lean and lean amine rate, the number of absorption stages and the semi-lean feed stage were varied. A lower equivalent heat than 2.90 MJ/kg CO$_2$ (as for the vapour recompression case) was however not achieved.

2.5. Simulation strategy and calculation sequence

The simulation strategy and calculation sequence were based on earlier work at Telemark University College by Øi [13], Øi and Vozniuk [10] and Øi and Shchuchenko [11]. The calculation sequence in Aspen HYSYS was based on initial estimates of flow rates and compositions to the absorption column for initial conditions. In the case of vapour recompression and recirculation to the desorber column, the flow rate, temperature and compositions from the compressor to the desorber also had to be estimated for initial conditions.
In the calculation sequence, the absorber was calculated first. Then the rich amine pump and the rich side of a multi-stream heat exchanger were calculated before the desorber. After the desorber and lean amine flash, the lean and semi-lean side of the multi-stream heat exchanger was calculated. The specified minimum temperature difference was achieved by adjusting (by an ADJUST block) the rich amine temperature to the desorber. Then the return pumps, the compressor and the coolers were calculated. The concentrations of the lean and semi-lean streams were then checked (in RECYCLE blocks) against the specified concentrations in the feed streams to the columns. The specified CO₂ removal grade of 85% was achieved by adjusting (by an ADJUST block) the lean amine circulation rate.

The convergence of the recycle blocks was improved when the total material balance of water and amine was fulfilled. This was performed in the simulations by adding make-up water and make-up amine (by SET calculation blocks) into the lean stream before the recycle blocks.

When the number of stages in the absorber was increased (above about 25 stages), problems with divergence occurred, as expected. Except for that, the flowsheets calculating split-stream or a combination of split-stream and vapour recompression had the most serious divergence problems. This is reasonable, because these flowsheets are complex and contain several recycle streams. The columns were calculated with the modified HYSIM inside out solver with adaptive damping, which in most cases gave the best convergence. Both the Kent-Eisenberg and the Li-Mather equilibrium models were tried. The experience was that Kent-Eisenberg was faster, while the Li-Mather calculations were more robust.

2.6. Energy comparisons of the alternatives

In Table 2 the equivalent heat (heat + 4 times compressor work) are listed for the four alternatives. The Li-Mather model was used in these calculations. The Kent-Eisenberg model gave slightly higher heat consumption.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard process</td>
<td>3.26</td>
<td>3.26</td>
<td></td>
</tr>
<tr>
<td>Split-stream</td>
<td>3.25</td>
<td>3.25</td>
<td></td>
</tr>
<tr>
<td>Vapour recompression</td>
<td>2.56</td>
<td>0.085</td>
<td>2.90</td>
</tr>
<tr>
<td>Vapour recompression + split-stream</td>
<td>2.81</td>
<td>0.053</td>
<td>3.02</td>
</tr>
</tbody>
</table>

The standard process gives a lower value than in most references [7,9,13,17], and as mentioned earlier, this can be explained by a high number of stages, a low temperature difference and a low removal grade.

For the split-stream process, the calculated value in this work is slightly higher than calculated by e.g. Øi and Voziuk [10] who calculated 3.0 MJ/kg CO₂ for a similar process. In that case, the number of stages was higher (24 stages).

The vapour recompression case has been calculated by Karimi et al. [9] who calculated a reboiler duty of 2.6 MJ/kg CO₂ using the program Unisim compared to a base case using 3.5 MJ/kg CO₂ captured from a coal based power plant. The values in this work are close to Karimi’s values. Using a rate-based simulation tool, a vapour recompression process has been calculated by Cousins et al. [7] with a reboiler duty of 3.0 MJ/kg CO₂ removed compared to a standard process using 3.8 MJ/kg CO₂. The reduction of 0.7 MJ/kg in this work is close to the reduction of 0.8 MJ/kg in Cousin’s work.

The configuration with vapour recompression and split-stream from the bottom of the desorber was simulated by Øi and Shchuchenko [11]. The reboiler duty was in that case calculated using the Kent-Eisenberg model to 2.45 MJ/kg CO₂ which in that work was slightly lower than for a simple vapour recompression case.
3. Dimensioning, cost estimation and optimization

3.1. Equipment dimensioning

The main equipment units have been dimensioned by traditional methods. In the absorber and the desorber, the diameters were calculated from gas velocities of 2.5 m/s and 1.5 m/s, respectively. One absorber stage with a Murphree efficiency of 0.15 was assumed to be equivalent to 1 meter of structured packing in the absorber. The overall heat transfer number in the rich/lean plate heat exchanger (or multi-stream heat exchanger) was estimated to 1000 W/(m²K), 1500 W/(m²K) was estimated for the shell and tube kettle reboiler. The efficiencies in the compressor and the pumps were 0.75. Other specifications are given in the Bachelor project report [12].

3.2. Operating cost

The electricity cost was specified to 0.068 USD/kWh and the steam cost was specified to 0.017 USD/kWh. The ratio between electricity and steam cost is 4. This is reasonable in a steam based power plant with a conversion efficiency of low pressure steam into electricity of approximately 25%. Operating time was set to 8000 hours/year.

Only the electricity consumption for the recompression was included. The differences in pump effects are assumed to be negligible. The exhaust gas fan is not included because the differences in pressure drop through the columns are assumed to be small.

3.3. Estimation of investment

Investment cost is calculated using methods from Turton et al. [18]. The bare module cost is calculated for each equipment unit. The bare module cost is the sum of direct and indirect expenses for the unit. Direct expenses are purchased cost and installation cost. Purchase cost is dependent on material of construction and pressure. Indirect expenses comprise engineering expenses, construction overhead, freight, insurance and tax. Bare module cost was calculated in USD (2001) and converted to USD (2011) using the Chemical Engineering Plant Cost Index (CEPCI). In cases where the range of cost correlations was exceeded, a cost exponent of 0.6 was used for capacity correlations for most equipment. For plate heat exchangers the exponent used was 1.0, indicating that the cost per m² does not decrease with size. This was assumed because the lean/rich heat exchanger is so large that it is expected to consist of several heat exchangers in parallel.

Net present value (NPV) using total cost (bare module cost and operating cost) was calculated for a period of 15 years with an effective discount rate of 10.5%. Table 3 shows net present value (negative) for different process configurations.

<table>
<thead>
<tr>
<th>Process configuration</th>
<th>Equivalent heat [MJ/kg]</th>
<th>NPV [mill. USD]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard process</td>
<td>3.26</td>
<td>550</td>
</tr>
<tr>
<td>Split-stream</td>
<td>3.25</td>
<td>603</td>
</tr>
<tr>
<td>Vapour recompression</td>
<td>2.90</td>
<td>513</td>
</tr>
<tr>
<td>Vapour recompression + split-stream</td>
<td>3.02</td>
<td>522</td>
</tr>
</tbody>
</table>
3.4. **Final optimization**

After concluding that the vapour recompression configuration was probably the most cost optimum process, the number of stages and minimum temperature difference were varied to find the most cost optimum process for the given specifications. First, the absorption column height (equivalent to the number of stages with a Murphree efficiency of 0.15) was optimized, and the optimum net present value was achieved with 16 stages. Then the total cost for different minimum temperature differences with 16 stages were calculated as shown in Fig. 7. The optimum was calculated to 12 K. With a heat exchanger cost exponent lower than 1.0, the optimum temperature difference was calculated to be lower.

It was concluded that the cost optimum case was a simple vapour recompression case with 16 meter packing height and minimum temperature difference 12 K.

![Fig. 7. Net present value (negative) as a function of minimum temperature difference for vapour recompression with 16 stages](image)

3.5. **Evaluation of uncertainty in dimensioning, investment, operating cost and total cost**

In the task to find a cost optimum configuration and cost optimum process conditions, the uncertainties in the process calculations are probably less than the uncertainties in dimensioning and cost estimation. The differences in calculated heat consumption in the literature for similar configurations are small.

The uncertainty in the cost of heat and work is considerable. The electricity cost is very case dependent, and the uncertainty in the heat (normally steam) cost is even larger. The uncertainty in energy cost is however probably lower than the uncertainty in investment.

There is high uncertainty in the dimensioning of the absorption column height and heat exchanger area. In this work, the number of absorption stages was held constant in most of the simulations, so the cost of the absorber packing should be about the same. The uncertainty in the heat exchanger size and cost will influence on the optimum minimum temperature difference. The uncertainty in the cost of a compressor for vapour recompression is large because this is probably not a standard compressor.

A vapour recompression process looks promising compared to a standard process because it achieves a large energy reduction, and compared to the other alternatives because it has a limited increase in complexity.
4. Conclusions

Different configurations for CO₂ capture at atmospheric pressure have been simulated in the process simulation tool Aspen HYSYS. It has been shown that it is possible to reduce the energy consumption considerably using a split-stream configuration or using vapour recompression. An energy reduction from 3.26 MJ/kg CO₂ in a standard process to an equivalent heat consumption of 2.90 MJ/kg CO₂ for a vapour recompression process has been calculated. It was not achieved any further reduction in equivalent heat consumption for a combination of a split-stream and vapour recompression process.

Operating cost for the different cases has been calculated, and a total cost evaluation has been performed for the most promising alternatives. The vapour recompression configuration was optimized with regard to the optimum net present value. For the vapour recompression configuration, 16 absorption stages and 12 K in minimum temperature difference was the calculated optimum.

The results of this work indicate that the vapour recompression configuration gives both the lowest energy consumption and the best net present value. There are still possibilities for optimization of the process. A process simulation tool like Aspen HYSYS combined with cost estimation is a reasonable tool for such optimization.

Acknowledgement

Thank you to Mohammed Ismail Shah, Gassnova, for help with information and suggestions for the work.

References