Comparison of energy consumption for different CO₂ absorption configurations using different simulation tools

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Abstract

The most studied method for CO₂ capture from exhaust gas is by absorption in an amine based solvent like monoethanolamine (MEA) followed by desorption. A drawback with this method is the large heat consumption needed for desorption. A reduction of this heat consumption using alternative configurations is possible. Different absorption and desorption configurations for 85 % CO₂ removal from a natural gas fired combined cycle power plant have been simulated with the process simulation tools Aspen HYSYS and Aspen Plus. In the Aspen Plus calculations, both an equilibrium based model including Murphree efficiencies and a rate-based approach were used. The results from this work show that all the simulation models calculate the same trends in the reduction of equivalent heat consumption when the absorption process configuration is changed from the standard process.

Keywords: absorption; CO₂; simulation; amine; efficiency

1. Introduction

Most studies on comparing different CO₂ absorption configurations are based on only one simulation tool and only one equilibrium model. It is of interest to find out whether the changes in heat consumption for alternative configurations are similar for different simulation tools and equilibrium models.

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Recent surveys on process flow-sheet modifications for energy efficient CO₂ capture from flue gas using chemical absorption have been published by Cousins et al. [1] and Le Moullec and Kanniche [2]. Rate-based Aspen Plus simulations for flow-sheet modifications like split-flow (split-stream) and vapour recompression processes have been performed and compared to a standard process by Cousins et al. [3]. Fernandez et al. [4] have performed cost estimation of the vapour recompression process based on Aspen Plus simulations and compared with a standard process. Simulations and cost estimation of several process modifications including split-flow and vapour recompression have been performed with the process simulation program Unisim by Karimi et al. [5]. Most of these comparisons have been performed on a CO₂ absorption process based on monoethanolamine. There has in general been published very few studies comparing different simulation tools for CO₂ absorption [6,7].

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 [8]. Øi and Shchuchenko [9] simulated different split-stream alternatives and vapour recompression alternatives also in Aspen HYSYS. Øi et al. [10] presented results from Aspen HYSYS simulations and cost estimation evaluations for different process configurations. Hansen [11] and Bergstrøm [12] have performed comparisons of CO₂ absorption simulations for different process configurations and different programs like Aspen HYSYS, Aspen Plus and ProMax. This is developed further in this work which is mainly based on the Master Thesis work by Kvam [13].

A traditional amine based CO₂ capture process has typically a reboiler heat consumption of 4.0 MJ/kg CO₂ captured. This has been minimized in several simulations with e.g. many absorption stages and a low minimum temperature difference for heat recovery to about 3.5 MJ/kg CO₂ [2,3,4,5,10]. Several of the references report simulated values of reboiler duty well below 3.0 MJ/kg CO₂ using e.g. the vapour recompression configuration. When the reboiler heat and compression work is combined to equivalent work or heat, typical reported values for equivalent heat consumption in improved configurations are in order of magnitude 3.0 - 3.5 MJ/kg CO₂.

2. Principles for vapour recompression and vapour recompression combined with split-stream

A standard amine based CO₂ capture process has a simple absorber and a desorber. A traditional configuration is shown in Fig 1. An amine solvent absorbs CO₂ in the absorber. The amine from the absorber (rich amine) is pumped through a heat exchanger to the desorber (stripper). Heat is added in the reboiler and cooling is performed in the top of the condenser. The regenerated bottom product of the desorber (lean amine) is pumped back through the amine/amine exchanger and a cooler to the absorber.

Fig. 1. Principle for a standard CO₂ removal process based on absorption followed by desorption in amine solution
Fig. 2 shows the principle for a vapour recompression configuration. The regenerated amine solution (lean amine in a traditional process) from the desorber is led through a pressure reduction valve to a flash tank (lean amine flash). The liquid from the flash tank (the lean amine) is recirculated back to the absorber. The vapour from the flash tank is compressed and returned to the bottom of the desorber.

![Fig. 2. Principle for a CO₂ capture process with vapour recompression](image1)

Fig. 3 shows the regeneration part of a process combining vapour recompression and split-stream. In a conventional split-stream process, a semi-lean amine stream from the middle of the desorber can be sent to the middle of the absorption column. The alternative shown in Fig. 3 takes the semi-lean stream from the bottom of the desorber as suggested by Øi and Shchuchenko [9]. 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) and the other part is sent to the lean amine flash where the liquid is sent to the top of the absorption column (as the lean stream). In Fig. 3 the flash gas to recompression is cooled in a multi-feed heat exchanger. This heat exchanger also involving both lean and semi-lean amine, will in practice consist of several heat exchangers.

![Fig. 3. Principle for a CO₂ absorption configuration with vapour recompression and split-stream from the bottom of the desorber](image2)
3. Different simulation tools and equilibrium models

3.1. Vapour/liquid equilibrium models

Aspen HYSYS has an amine package where the Kent-Eisenberg [14] and Li-Mather [15] equilibrium models are available. The column models in Aspen Plus are equilibrium based and can be specified with Murphree efficiencies on each stage. Aspen Plus has an Electrolyte-NRTL (Non-Random-Two-Liquid) equilibrium model which is based on Austgen et al. [16]. The column models can be specified with Murphree efficiencies and there is a rate-based column model available in Aspen Plus. Different equilibrium models used in process simulation of CO₂ absorption into amines are reviewed by Øi [17].

In Aspen HYSYS, the parameters in the amine package equilibrium models cannot be changed. In the Electrolyte-NRTL equilibrium model in Aspen Plus, the model parameters are in principle inserted by the user. There is an insert file available in the Aspen Plus program package containing a complete set of parameters for the Electrolyte-NRTL model. The parameter set in version 7 was updated compared to earlier versions. An example file for a rate-based CO₂ absorption process using MEA is also available in the Aspen Plus program package. The Electrolyte-NRTL parameters in the example file are not the same as in the insert file. It is commented by Liu [18] that the early versions of El-NRTL in Aspen Plus based on original parameters calculate too high reboiler duty.

3.2. Murphree efficiency

The principle of the definition of Murphree efficiency based on the gas phase mole fraction (y) for a trayed column is shown in Fig. 4. For a packed column, a tray in Fig. 4 can represent a packing height section.

![Fig. 4. Illustration of the definition of Murphree efficiency, \( E_M = \frac{(y - y_{n+1})}{(y^* - y_{n+1})} \), where \( y^* \) is in equilibrium with the liquid on stage n.](image)

Using Murphree efficiencies is a simple way to make a more realistic description of the concentration and temperature profiles as a function of column height compared to only using ideal equilibrium stages. When specifying Murphree efficiencies in process simulation programs, it is assumed that the gas and liquid temperatures are equal at each stage. A Murphree efficiency can be specified to e.g. 0.25 for every stage which is equivalent to order of magnitude 1 to 2 meter of packing height. Murphree efficiencies can be estimated automatically for each of the trays in the Aspen HYSYS program. Øi [7,17] has calculated estimated Murphree efficiencies as a function of temperature for CO₂ absorption into MEA for typical column top and column bottom conditions.
3.3. Rate-based simulation

A rate-based model simulates an absorption column by separating the liquid and vapour flow in the column and is based on the calculation of the heat and mass transfer rates between the phases combined with chemical kinetics. Some process simulation programs like Aspen Plus and ProMax can perform rate-based simulations. In Aspen Plus, there are several models available for heat transfer, mass transfer and kinetics which can be included in a rate-based simulation. A rate-based simulation in Aspen Plus needs several parameters in addition to the parameters in the Electrolyte-NRTL equilibrium model. A rate-based example file for CO₂ removal using MEA is available in the Aspen Plus program package.

4. Specifications and simulations

4.1. Specifications for base-case calculations

The specifications for a base-case simulation of a process as in Fig. 1 are given in Table 1. Most of the specifications are the same as in an earlier Aspen HYSYS simulation from Øi [19]. An absorption unit calculation based on equilibrium stages with Murphree efficiencies only need specifications for the number of stages, the Murphree efficiencies on each stage and a pressure profile in addition to the inlet streams. The Murphree efficiencies for the components except from CO₂ were set to unity.

In the Aspen HYSYS calculations, the vapour/liquid equilibrium models Kent-Eisenberg and Li-Mather were used with non-ideal gas. The equilibrium model used in Aspen Plus was Electrolyte-NRTL. In the equilibrium based calculations the Electrolyte-NRTL insert file in Version 7.2 was used.

The rate-based Aspen Plus simulations were based on an example file from the Aspen Plus program package (Rate_Based_MEA_Model in Version 7.2). Most of these specifications were also used by Zhang et al. [20] in their Aspen Plus rate-based simulation of CO₂ absorption. Some parameters were changed from the rate-based example file. The selected packing in both the absorber and desorber was standard metal Mellapak 250Y and the interfacial area factor was set to 1.0, and the height of each of 10 stages was 1.2 meter. The stage flow option was changed from countercurrent to mixed, which simulates both the vapour and the liquid as ideally mixed at each stage.

The calculation sequence in the Aspen HYSYS simulation was similar to the sequence in Øi [19]. The liquid stream including flow rate and concentrations to the absorber had to be guessed prior to the calculation of the absorber. The amine flow was then adjusted to achieve 85 % CO₂ removal. After the pump, the cold side of the amine/amine heat exchanger was calculated based on a guessed temperature on the stream to the desorber. After the desorber, the lean amine pump and the hot side of the heat exchanger was calculated. The temperature to the desorber was then adjusted to achieve 5 °C as the minimum temperature difference in the heat exchanger. The lean amine and some water was added to the liquid circulation to make up for the losses. The calculated recycle stream after the amine cooler was compared with the guessed stream and a recycle block was used to perform iterations to achieve convergence.

In the Aspen Plus simulations, the calculation sequence was slightly different, partly because the reboiler temperature in the desorber was not specified explicitly. In the equilibrium based simulation, a design spec was used to achieve 120 °C in the reboiler by varying the specified vapour flow out from the top of the desorber. Then the liquid flow (to the absorber) was varied to achieve 85 % CO₂ removal. It was checked manually that the lean amine recycle stream back to the absorber was equal to the specified flow to the absorber. In the rate-based simulation, the achieved reboiler temperature was 123 °C with a specified distillate flow (top product) of 6400 kmole/h.
Table 1. Specifications for base-case CO₂ removal

<table>
<thead>
<tr>
<th>Specified parameter [dimension]</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO₂ removal grade [%]</td>
<td>85</td>
</tr>
<tr>
<td>Inlet absorber gas/ liquid temperature [ºC]</td>
<td>40</td>
</tr>
<tr>
<td>Inlet gas pressure [bar (a)]</td>
<td>1.1</td>
</tr>
<tr>
<td>Inlet gas flow [kmol/h]</td>
<td>85000</td>
</tr>
<tr>
<td>CO₂ in inlet gas [mol-%]</td>
<td>3.73</td>
</tr>
<tr>
<td>Water in inlet gas [mol-%]</td>
<td>6.71</td>
</tr>
<tr>
<td>Minimum temperature difference [ºC]</td>
<td>5</td>
</tr>
<tr>
<td>Lean amine pressure [bar (a)]</td>
<td>1.0</td>
</tr>
<tr>
<td>Lean amine rate [kmole/h] (in first iteration)</td>
<td>120000</td>
</tr>
<tr>
<td>MEA in lean amine [mass-%] (first iteration)</td>
<td>29</td>
</tr>
<tr>
<td>CO₂ in lean amine [mass-%] (first iteration)</td>
<td>5.5</td>
</tr>
<tr>
<td>Number of stages in absorber</td>
<td>10</td>
</tr>
<tr>
<td>Murphree efficiency in absorber</td>
<td>0.25</td>
</tr>
<tr>
<td>Pump adiabatic efficiency</td>
<td>0.75</td>
</tr>
<tr>
<td>Number of equilibrium stages in desorber</td>
<td>6</td>
</tr>
<tr>
<td>Desorber pressure [bar]</td>
<td>2.0</td>
</tr>
<tr>
<td>Reboiler temperature [ºC]</td>
<td>120</td>
</tr>
<tr>
<td>Reflux ratio</td>
<td>0.3</td>
</tr>
</tbody>
</table>

4.2. Specifications of vapour recompression calculations

A vapour recompression process as in Fig. 2 was simulated. The pressure in the lean amine flash was first specified to 1.2 bar. The adiabatic efficiency in the compressor was specified to 75 %. The vapour recompression simulation had 15 absorption column stages compared to 10 in the base-case simulation. The number of stages was increased because in the case of vapour recompression and especially when including split-stream, it is possible to make a benefit out of an increased number of stages. Except for that, most of the specifications in Table 1 were used. After iteration, the obtained lean loading was lower in the vapour recompression case compared to the base-case.

Equivalent heat consumption was calculated as reboiler duty + 4 times the compressor work to compare heat consumptions. Energy as work will have a higher value or cost compared to energy as heat. Other references use similar values for conversion between compressor work and reboiler duty. Le Moullec and Kanniche [2] used 3.57 (1/0.28) and Fernandez et al. [4] used 4.35 (1/0.23). These values are based on the assumption that the steam used for reboiler heat can be converted to work in a steam turbine with an efficiency of about 0.25.

The calculation sequence in the case of vapour recompression is only slightly more complicated than in the base-case. To calculate the desorber the first time, the flow and the conditions of the flash gas has to be guessed. After the desorber, the lean vapour flash is calculated, and the desorber can be recalculated. In the Aspen HYSYS simulation, this iteration is performed by a recycle block. In Aspen Plus, the iterations were performed manually by insertion.

In the Aspen Plus simulation, the calculation sequence was based on the same principles as in the base-case. Results for both the Aspen Plus equilibrium simulation and the Aspen Plus rate-based simulation were obtained.
4.3. Specifications for vapour recompression combined with split-stream

A combined process with vapour recompression and split-stream as in Fig. 3 was simulated. The flash pressure was 1.2 bar as in the vapour recompression case. The number of absorption stages was 15. The semi-lean amount and the feed stage to the absorber was specified to a constant value and later varied to minimize the reboiler duty. Except for this, the specifications in Table 1 were used. However, the CO₂ concentration (loading) of semi-lean and lean amine to the absorber had to be adjusted after some iterations.

The calculation sequence in the case of the combination of split-stream and vapour recompression is more complicated than in the other cases. 3 recycle blocks were used in the Aspen HYSYS calculation. Before the absorber can be calculated, both the lean and semi-lean stream has to be guessed. As in the vapour recompression case, the flash gas amount to the desorber had to be guessed, and a recycle block is used for iteration. After one iteration, the semi-lean amine amount and concentration was fixed. Then the lean amine rate (and concentration) was varied to achieve 85 % CO₂ removal. The iteration process was in this case quite complex. Results were obtained only for the Aspen HYSYS and Aspen Plus equilibrium simulation for the combined process. Convergence was not achieved for the rate-based simulation.

5. Results and discussion

5.1. Summary of results

In Table 2 the equivalent heat (heat + 4 times compressor work) are listed for the most important alternatives.

<table>
<thead>
<tr>
<th>Simulation tool / Equilibrium model</th>
<th>Standard process 10 absorber stages (base-case)</th>
<th>Vapour recompression (reboiler duty)</th>
<th>Vapour recompression (equivalent heat)</th>
<th>Vapour recompression with split-stream</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aspen HYSYS / Kent Eisenberg</td>
<td>3.48</td>
<td>2.75</td>
<td>2.98</td>
<td>3.12</td>
</tr>
<tr>
<td>Aspen HYSYS / Li-Mather</td>
<td>3.42</td>
<td>2.66</td>
<td>2.92</td>
<td>3.03</td>
</tr>
<tr>
<td>Aspen Plus Equilibrium / Ei-NRTL</td>
<td>3.37</td>
<td>2.95</td>
<td>3.13</td>
<td>3.17</td>
</tr>
<tr>
<td>Aspen Plus Rate-based / Ei-NRTL</td>
<td>4.26</td>
<td>3.57</td>
<td>3.82</td>
<td>Not converged</td>
</tr>
</tbody>
</table>

5.2. Evaluation of the base-case calculations

The heat consumption for the standard process was calculated in the range from 3.37 to 4.26 MJ/kg CO₂. The Aspen Plus equilibrium model calculated the lowest heat consumption while the Aspen Plus rate-based model calculated the highest. The heat consumption calculated with Aspen HYSYS using the Kent-Eisenberg and Li-Mather models were slightly higher than the values calculated with the Aspen Plus equilibrium model using Electrolyte-NRTL. This indicates that the differences in calculated heat consumption are due to differences between parameters in the equilibrium models. It is assumed that the parameters in the Aspen Plus Electrolyte-NRTL models are different because different sources were probably used in the insert file and the example file.

The standard process gives a slightly lower value than in most other references [2,3,4,5]. This can be explained by a low temperature difference in the amine/amine heat exchanger and a low removal grade. Similar values as in these calculations were calculated in Aspen HYSYS simulations by Øi et al. [10] achieving 3.65 with 10 K temperature difference in the amine/amine heat exchanger using the Kent-Eisenberg model and 3.4 MJ/kg CO₂ using the Li-Mather model with 82 % removal grade.
Kothandaraman [21] calculated the heat consumption for typical conditions using Aspen Plus. 4.3 MJ/kg CO2 was achieved using an equilibrium based model and 4.5 MJ/kg CO2 was achieved using a rate-based model. Bergstrøm [12] simulated both equilibrium based and rate-based simulations with the equilibrium model from the Aspen Plus rate-based example file. Then the reboiler duty was calculated to 4.5 MJ/kg CO2 for the equilibrium model using Murphree efficiencies and 4.4 in the rate-based calculations. The high values are probably due to the Electrolyte-NRTL version used. As mentioned earlier, it is well known that the earlier Electrolyte-NRTL calculations gave higher heat consumptions compared with newer versions [18]. Fernandez et al. [4] using Aspen Plus Version 7.1, used 3 equilibrium stages in the absorber and calculated a reboiler heat consumption of 3.56 MJ/kg CO2. Karimi et al. [5] using Unisim (a version of Aspen HYSYS) calculated 3.54 MJ/kg CO2. Unisim has the same amine package as Aspen HYSYS with the Kent-Eisenberg and the Li-Mather model.

5.3. Evaluation of vapour recompression calculations

The reboiler heat consumption for the vapour recompression process from Table 2 was calculated in the range from 2.66 to 3.57 MJ/kg CO2. The reduction in reboiler duty varied between 0.42 and 0.76 MJ/kg CO2. The equivalent heat consumption for the vapour recompression process was calculated in the range from 2.92 to 3.82 MJ/kg CO2. The reduction in equivalent heat consumption varied between 0.24 and 0.50 MJ/kg CO2.

The vapour recompression case has been calculated by Karimi et al. [5] who calculated a reboiler duty of 2.60 MJ/kg CO2 using the program Unisim compared to a base case using 3.54 MJ/kg CO2 captured from a coal based power plant. The values from Aspen HYSYS in this work are close to Karimi’s values. Using a rate-based simulation tool (not specified), a vapour recompression process has been calculated by Cousins et al. [3] with a reboiler duty of 3.04 MJ/kg CO2 removed compared to a standard process using 3.75 MJ/kg CO2. The reduction in this work is close to the reduction of 0.71 MJ/kg in Cousin’s work. Fernandez et al. [4] using an Aspen Plus equilibrium model calculated a vapour recompression process at a 1.2 bar flash pressure and desorption pressure of 1.8 bar. A reboiler duty of 3.03 MJ/kg and equivalent heat consumption of 3.30 MJ/kg was calculated with the conversion factor 4.35 (1/0.23) between work and equivalent heat. Aspen Plus equilibrium calculates also here a smaller improvement compared to using Kent-Eisenberg and Li-Mather in Aspen HYSYS.

The pressure in vapour recompression was varied, and the equivalent heat was calculated. The energy optimum pressure was calculated to be between 1.0 and 1.2 bar for the Kent-Eisenberg model, between 1.1 and 1.2 bar for the Li-Mather model, at 1.2 bar for the Aspen Plus equilibrium model and between 1.0 and 1.1 bar for the Aspen Plus rate-based model. These values (all between 1.0 and 1.2) are close to literature values at 1.1 bar from Karimi et al., 1.2 bar from Fernandez et al. and 1.25 from Le Moullec and Kanniche. The highest value from Le Moullec and Kanniche was for a high desorption pressure of 2.5 bar.

The simulations of vapour recompression were performed without cooling of the flash gas before compression. The temperature increased to about 170 °C after compression. MEA may degrade at temperatures above 130 °C. There are two advantages with cooling, the compressor work will be reduced and high temperatures will be avoided. In the simulations combining vapour recompression and split-stream, cooling of the flash gas was performed. The simulations showed that cooling to avoid temperatures above 120 °C had a very minor influence on the calculated compressor duty and equivalent heat.

5.4. Evaluations of vapour recompression combined with split-stream

The equivalent heat consumption for the vapour recompression combined with split-stream was calculated in the range from 3.03 to 3.17 MJ/kg CO2. The reduction in equivalent heat consumption varied between 0.20 and 0.36 MJ/kg CO2. Aspen HYSYS with the Li-Mather model calculated the lowest heat consumption for these configurations while the Aspen Plus rate-based model calculated the highest. This indicates that the combination of vapour recompression and split-stream does not achieve a lower equivalent heat compared to the simple vapour recompression case. An advantage for the combined configuration is that the compressor size decreases. The more complex process is however probably a more important disadvantage.
Øi et al. [10] presented results from simulations using Aspen HYSYS for vapour recompression combined with split-stream. Also in this work, it is shown that the simple vapour recompression configuration gives slightly lower equivalent heat. It might be possible to reduce the heat consumption in the combined process by reducing the accepted temperature difference in the amine/amine heat exchanger to below 5 °C.

5.5. Further discussion

All the tools and equilibrium models gave approximately the same results, except for the rate-based simulation which calculated significantly higher heat consumption for all cases. The main reason for the difference is probably that different versions of the Electrolyte-NRTL equilibrium model are used. The Aspen Plus equilibrium model with the updated parameters gives the lowest reduction. The reboiler heat calculated by the Aspen Plus Electrolyte-NRTL equilibrium model is very close to Kent-Eisenberg and Li-Mather for the standard model. All the simulation tools are suitable to simulate different process configurations for comparisons. The Aspen Plus rate-based tool is the most detailed and the most challenging tool.

All the models calculate the same trends in the reduction of equivalent heat consumption when the absorption process configuration is changed from the standard process. All the simulation models calculate that the reduction is higher for a vapour recompression process than for a split-stream process or a vapour recompression process combined with split-stream. The results show that the vapour recompression process is a reasonable configuration for reducing the energy consumption in a CO2 absorption process.

Simulations with Murphree efficiencies and rate-based simulation gave different results in some cases. It is not obvious whether using Murphree efficiencies or a rate-based model gives most accurate results. An advantage using Murphree efficiencies in CO2 absorption simulations is that it is simple and robust. An advantage using rate-based simulations is that it can take into consideration more detailed effects of equilibrium, kinetics, heat and mass transfer.

6. Conclusions

Different CO2 capture process configurations based on MEA absorption have been simulated with Aspen HYSYS and Aspen Plus with rate-based simulations and simulations with specified Murphree efficiencies. The rate-based simulations calculated higher heat consumption compared to the simulations based on Murphree efficiencies. The reduction of heat consumption from a base-case configuration to a vapour recompression configuration was however similar independent on equilibrium model or whether the simulation was equilibrium based or rate-based.

The results from this work show that all the simulation models calculate the same trends in the reduction of equivalent heat consumption when the absorption process configuration is changed from the standard process. All the simulation models calculate that the reduction is higher for a vapour recompression process than for a vapour recompression process or a vapour recompression process combined with split-stream. The results show that the vapour recompression process is a reasonable configuration for reducing the energy consumption in a CO2 absorption process.

References


