Process Simulation, Cost Estimation and Optimization of CO_2 Capture using Aspen HYSYS

Lars Erik Øi* Nils Eldrup Solomon Aromada Andrea Haukås Joakim Helvig
Ida Hæstad Anne Marie Lande

Department of Process, Energy and Environmental Technology, University of South-Eastern Norway
Corresponding author's email address: lars.oi@usn.no

Abstract

A standard method to remove CO_2 is by absorption in monoethanol amine (MEA) followed by desorption. A traditional aim has been to find the process parameters which give the lowest combined investment and operating cost. The aim in this work is to calculate cost optimum process parameters and evaluate whether it is possible to perform automated cost estimation and optimization. Aspen HYSYS simulations of a standard amine based process for CO_2 capture from a cement plant have been performed. The capital cost of CO_2 capture was estimated based on equipment cost from Aspen In-plant cost estimator and a detailed factor method. Operating cost included electricity, heat consumption and maintenance. Optimum temperature difference in the main heat exchanger was calculated to 13 °C after one simulation for each temperature. The lowest calculated cost was achieved with 12 stages (meter packing height) based on one simulation for each stage number. With improved robustness of the simulations, it should be possible to optimize the temperature difference in one automated calculation. To optimize the height of the absorption column automatically, a way to update the number of stages during the simulations has to be found.

Keywords: carbon capture, Aspen HYSYS, simulation' cost estimation

1 Introduction

The cement industry accounts for more than 5 % of the total anthropogenic emissions of CO_2 in the world today (Norcem, 2019). There are several possible options to reduce emissions in the cement industry, one of them is CCUS (carbon capture, utilization and storage). Absorption using amine solutions is considered the most favorable method for capture of CO_2 from exhaust gas.

This work is based on the project work from Haukås et al. (2019) at the University of South-Eastern Norway (USN). It is a continuation of previous work at Telemark University College (TUC) and USN. This work has involved process simulation, equipment dimensioning, cost estimation and cost optimization of CO_2 capture. The simulation tool Aspen HYSYS has been used in most of the work, with the application of the amine package and constant stage (Murphree) efficiencies in the absorber and desorber.

1.1 Aim

The general aim of this project is to develop further models in Aspen HYSYS for calculation, equipment dimensioning, cost estimation and optimization of CO_2 capture by atmospheric exhaust gas absorption into an amine solution. The intention is to streamline the cost estimation and optimization procedure by utilizing the spreadsheet function in Aspen HYSYS. One specific aim is to calculate cost optimum process parameters and evaluate whether it is possible to perform automated cost estimation and optimization.

1.2 Literature

The combination of process simulation and cost estimation is an important tool to evaluate different CO_2 capture technologies (Rao and Rubin, 2002; Øi, 2012; Ali, 2019).

This work is a continuation of previous work of students at TUC and USN. In particular, the work is based on the master project from 2015 (Park et al., 2015), as well as the master thesis (Kallevik, 2010).

The project from 2015 involved process simulation, dimensioning and cost estimation of CO_2 capture from a cement plant with the use of Aspen HYSYS. MEA was the sorbent, and the amine package in Aspen HYSYS was applied. Capture rate, energy demand per kg CO_2 captured, and capture cost per ton CO_2 were calculated. The base case had a CO_2 removal efficiency of 90 %. The Aspen HYSYS simulation performed in 2015 did not have any adjust operations incorporated.

In the master's thesis by Kallevik (2010), a simulation and cost estimation of a carbon capture process was developed in Aspen HYSYS in an attempt to cost optimize the process. By varying the removal efficiency and changing process parameters, such as minimum temperature difference in the main heat exchanger, an optimum solution for the minimum temperature difference was found.

The thesis by Kallevik used the amine package for his simulations in Aspen HYSYS. In addition, an adjust operation was implemented in the flowsheet in order to get an automated model to specify the minimum approach temperature in the heat exchanger.

1.3 Process description

Figure 1 shows a standard process for CO_2 absorption into an amine-based solvent. It comprises an absorption column, a stripping column including a reboiler and condenser, circulating pumps and heat exchangers. The process is described in more detail in Kallevik (2010) and Øi (2012).

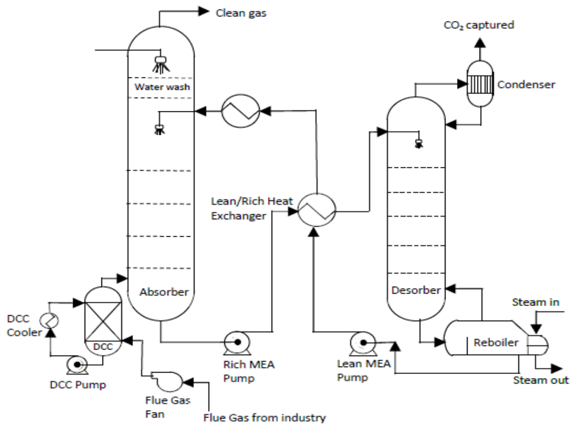

Figure 1. Process flow diagram of a standard amine-based CO_2 capture process

2 Methodology

The process simulation tool Aspen HYSYS version 10 was used for all the simulations performed in this report. The amine package (which is now the recommended equilibrium model by Aspen HYSYS) and constant Murphree efficiencies were specified in the absorber and desorber.

2.1 Specifications and simulation of standard CO_2 capture process

The specifications in Table 1 correspond to 90 % CO_2 removal efficiency and a minimum approach temperature of 10 °C in the lean/rich heat exchanger. This is the base case alternative.

The calculation sequence is similar to earlier works (Aromada and Øi, 2015). Even though Aspen HYSYS is an equation based program, the calculation strategy is based on a sequential modular approach (Kisala et al., 1987; Ishii and Otto, 2008). First the absorption column is calculated from the inlet gas and the lean amine (which is first guessed). The rich amine from the bottom of the absorption column passes through the pump and the rich/lean heat exchanger. The temperature after the heat exchanger is specified. The heated rich amine is entering the desorption column which calculates the CO_2 product and the hot lean amine. The hot lean amine is pumped to a higher pressure in a pump, passes through the lean/rich heat exchanger and is further cooled in the lean cooler. Then this lean amine is checked in a recycle block. It is checked whether the flow and composition in the recycled lean amine is sufficiently close to the earlier guessed lean amine stream, which may be changed by iteration.

Two adjust operations were implemented in the flowsheet in order to get an automated simulation model. One is adjusting the minimum approach temperature in the lean/rich heat exchanger and another adjusting the removal efficiency based on the lean amine mass flow. The process flowsheet is shown in Figure 2.

Table 1. Aspen model parameters and specifications for the base case alternative

Parameter	
Inlet flue gas temperature [°C]	40.0
Inlet flue gas pressure [kPa]	110.0
Inlet flue gas flow rate [kmol/h]	8974
CO_2 content in inlet gas [mole %]	17.8
Water content in inlet gas [mole %]	19.5
Lean amine temperature [°C]	45.0
Lean amine pressure [kPa]	101.0
Lean amine rate [kg/h]	$1.103 \cdot 10^6$
MEA content in lean amine [mass %]	28.71
CO_2 content in lean amine [mass %]	5.16
Number of stages in absorber [-]	10
Murphree efficiency in absorber [m^{-1}]	0.15
Rich amine pump pressure [kPa]	220.0
Rich amine temp. out of HEX [°C]	102.8
Number of stages in desorber [-]	6
Murphree efficiency in desorber [m^{-1}]	1.0
Reflux ratio in stripper [-]	0.3
Reboiler temperature [°C]	120.0
Lean amine pump pressure [kPa]	200.0

2.2 Parameter variations

Three different parameters were varied in order to study the effects on the cost estimate:

1. Minimum approach temperature in lean/rich heat exchanger
2. CO_2 removal efficiency
3. Number of stages in the absorber

10 stages, removal efficiency of 90 % and a 10 °C minimum approach temperature correspond to the base case simulation. In the additional cases, all the base case parameters were constant except the parameter to be optimized.

2.3 Process convergence and tolerances

To converge a column model in a simulation software tool, e.g. Aspen HYSYS, all equations describing equilibrium, gas and liquid flow must be solved for each calculation stage. Aspen HYSYS has a default set of criterias for converging of column models, and also preset calculation parameters. References for flow-sheet convergence and stage-to-stage column convergence are Kisala et al. (1987), Ishii and Otto (2008) and Holoboff (2020).

In order to achieve convergence, there are different calculation models available in Aspen HYSYS. In the columns, the best convergence is achieved by using the Modified Hysim Inside-Out algorithm with adaptive damping in absorber and desorber (Øi, 2012).

Aspen HYSYS is an equation-based simulation software, which means that it has the ability to calculate in-streams based on out-streams. However, the calculation strategy in this work is sequential. In the case of recycle streams, one must include recycle blocks to solve the flowsheet in Aspen HYSYS. This block compares the in-stream to the block with the out-stream from the block with the previous iteration.

The goal of tolerance testing is to reach a specified target value with an accuracy up to a certain number of decimals. An investigation of the column and flowsheet convergence in the base case simulation was performed by decreasing the tolerances of the adjust operations. The secant method in Aspen HYSYS was applied for all alternatives.

In order to reach the target value of minimum approach temperature equal to 10 °C, the temperature of rich amine out of the heat exchanger was varied with the adjust operation. Each new trial had a more restrictive tolerance than the previous.

The varied parameter in the testing of the removal efficiency is the mass flow of the lean amine into the absorber. The target value is a cleaning efficiency of 90.00 % that is calculated from the molar flow of CO_2 in the cleaned gas out of the absorber.

The tolerance of the recycle operation was also decreased. In the recycle operation the tolerance of various parameters like temperature, pressure, flow, composition and individual components can be modified independently.

2.4 Dimensioning and cost estimation calculations

The following procedure was implemented for the cost estimation:

1. Simulation of the CO_2 capture process in Aspen HYSYS with the base case specifications in Table 1.
2. Dimensioning of the equipment based on the simulation result
3. Calculation of equipment cost for each unit using Aspen In-Plant cost estimator
4. Calculation of installation cost based on a detailed factor table. The factor was kept constant under parameter variation
5. Correction of currency and index
6. Estimation of annual operational costs based on energy requirement from the simulation result
7. Calculation of net present value based on a given discount rate and project lifetime
8. Calculation of CO_2 capture cost for comparison between the different case simulations

2.4.1 Scope analysis

The cost analysis is limited to the equipment listed in the flow-sheet in Figure 1 excluding the flue gas cooler. No pre-treatment like inlet gas purification or cooling is considered, and no treatment after stripping like compression, transport or storage of CO_2 is considered. The cost estimate is limited to installed cost of listed equipment. It does not include e.g. land procurement, preparation, service buildings or owners cost.

2.4.2 Dimensioning of equipment

For the absorber and desorber internals, a structured packing was chosen because it yields a low pressure drop, high efficiency and high capacity (Øi, 2012). To determine the packing height, a constant stage (Murphree) efficiency corresponding to 1 meter of packing was assumed. Murphree efficiencies of 0.15 and 1.0 were specified for the absorber and the desorber in Table 1.

Centrifugal pumps with 75 % adiabatic efficiency were used in the process simulation. The pump duties that are calculated by Aspen HYSYS does not take the lifting height into consideration, only the pressure difference across the pump. Since the pumps are not the most expensive equipment in a CO_2 capture plant, an approximate additional duty compensating for the lifting height was included.

The absorption column diameter was calculated based on a gas velocity of 2.5 m/s and the desorption column is based on a gas velocity of 1 m/s as in Park and Øi (2017). The packing height of the absorption and desorption column is 1 meter per stage with a specified stage efficiency. The total height of the absorption column and desorption column is specified to be 40 m and 16 m respectively. The extra height is due to distributors, water wash packing, demister, gas inlet, outlet and sump.

Overall heat transfer coefficient values have been specified for lean/rich heat exchanger 550 W/(m^{2}K), lean amine cooler 800 W/(m^{2}K), reboiler 2500 W/(m^{2}K) and condenser 2000 W/(m^{2}K). These values are higher than in Øi (2012) and Park and Øi (2017) which are regarded as conservative.

2.4.3 Capital cost estimation methods

Table 2 specifies general assumptions made for the cost comparison.

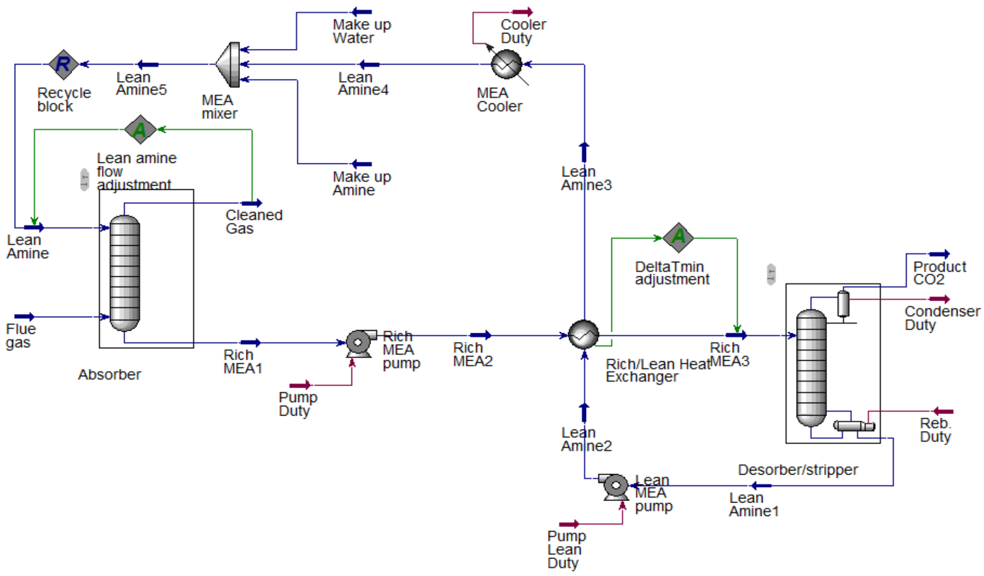

Figure 2. Aspen HYSYS flow-sheet of the base case simulation

The equipment costs are taken from the Aspen In-plant Cost Estimator (v.10), which gives the cost in Euro (€) for Year 2016 (1st Quarter). A generic location that has good infrastructure and easy access to a workforce and materials, e.g. Rotterdam, is assumed. Stainless steel (SS316) with a material factor of 1.75 was assumed for all equipment units.

In the detailed factor method, each equipment cost (in carbon steel) was multiplied with its individual installation factor to get equipment installed cost, as in earlier works (Øi, 2012; Park and Øi, 2017). The total capital cost was then calculated by adding all the individual equipment installed costs. The detailed installation factor is a function of the site, equipment type, materials, size of equipment and includes direct costs for erection, instruments, civil, piping, electrical, insulation, steel and concrete, engineering cost, administration cost, commissioning and contingency. The updated installation factors for year 2016 (Eldrup, 2016) were used.

Table 2. Cost calculation specifications

Parameter	Value
Plant lifetime	20 years
Discount rate	7.5 %
Maintenance cost	5 % of installed cost
Electricity price	0.5 NOK/kWh
Steam price	0.13 NOK/kWh
Annual operational time	8000 hours
Location	Rotterdam
Currency exchange rate 2016	9.209 (European Central Bank, 2019)
Cost index 2016	103.6 (Statistics Norway, 2019)
Cost index September 2019	111.1

This cost estimate is expected to have an accuracy of ±40%.

2.4.4 Operating cost calculation

The sum of all the costs for running the project is calculated to be the total OPEX per year. This project includes OPEX estimations for the use of electricity and steam to run the CO_2 capture process. Electricity cost was specified to be 0.5 NOK/kWh (approximately 0.05 Euro/kWh). The steam cost was specified to be 25 % of the electricity cost, 0.125 NOK/kWh. Running uptime for the project was assumed to be 8000 hours.

2.4.5 Aspen HYSYS spreadsheet calculations.

The spreadsheet unit in Aspen HYSYS was used to calculate the detailed cost estimation of CAPEX, OPEX and NPV (net present value). The NPV was calculated as the sum of CAPEX and OPEX for a calculation period of 20 year, and with discount factor 7.5 % as specified in Table 2.

For the different alternatives (especially when varying the parameters to be optimized) the spreadsheet calculated the NPV for each set of alternative parameter values.

For the case of optimizing the temperature difference in the main heat exchanger, the calculation could be made effectively by using a Case Study option in Aspen HYSYS, so that the calculations could be performed automatically for each pre-selected parameter value.

For the case of optimizing the number of absorber stages, each calculation was performed independently by specifying the number of stages in each calculation. The optimum number of stages can then be found as the number giving the lowest NPV.

3 Results and Discussion

3.1 Simulations and convergence

The calculation sequence including the recycle block and the adjust operations were developed as a result of a combination of earlier work and trial and error. The recycle block did not converge without adjusting the makeup water (and makeup amine). This was done manually or it was calculated by a material balance. An improved procedure for the calculation of the water (and amine) makeup can probably increase the convergence efficiency.

The DeltaTmin adjust block was efficient to find the specified minimum temperature approach in the main heat exchanger. When the tolerance was reduced, more iterations (than the specified) was often necessary to achieve convergence. The Lean amine flow adjust block was the most difficult to converge. This can be explained by that the recycle block had to be solved for each iteration. The recycle block was difficult to converge by itself, and the variation of the amine flow to obtain the specified CO_2 removal grade made the convergence more difficult. When the tolerance was reduced, the number of iterations both in the recycle block and in the adjustment operation increased.

3.2 General optimization results

The results given in Figure 3, Figure 4 and Figure 5 are similar to results in an earlier report (Park et al. 2015) with similar conditions. The optimum parameter values are also close to values from earlier work (Kallevik, 2010; Øi, 2012; Aromada and Øi, 2017). Some test calculations indicate that the change in equilibrium model in Aspen HYSYS to the acid gas package, does not change the results much.

3.3 Optimum number of stages

Figure 3 shows the energy consumption (in MJ/kg CO_2 captured) and negative NPV (in mill. NOK) for the number of stages 8, 10 and 12.

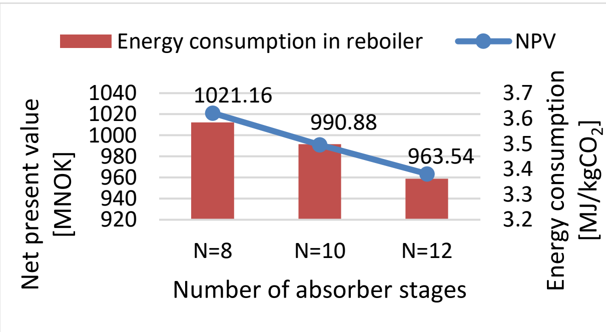

Figure 3. Energy consumption and negative net present value for the number of stages case simulations.

The figure shows that the energy consumption decreases significantly when the number of stages increases. It also shows that the NPV becomes less negative as the number of stages increases. The decrease from 10 to 12 stages is only 3 %. This indicates that the optimum is slightly higher than 12. To optimize the number of stages, it is necessary to start a new calculation for every specified number of stages.

3.4 Optimum minimum T approach

Figure 4 shows the energy consumption (in MJ/kg CO_2 captured) and negative NPV (in mill. NOK) for the minimum temperature approach in the main amine heat exchanger equal to 5, 10, 13 and 15. The figure shows that the energy consumption increases significantly when the minimum temperature difference increases. It also shows that the NPV is very little dependent on the minimum temperature approach. When the conditions are changed slightly, the optimum temperature approach changes between approximately 10 - 15 °C. This is similar to results from other work. To optimize the minimum temperature, the most efficient way found, is to perform a Case Study in Aspen HYSYS. Then the optimum value can be found as the one with minimum (negative) NPV. In principle, the optimization could be performed by adding a minimization procedure in the Aspen HYSYS spreadsheet, and return a next minimum temperature approach to the Aspen HYSYS program.

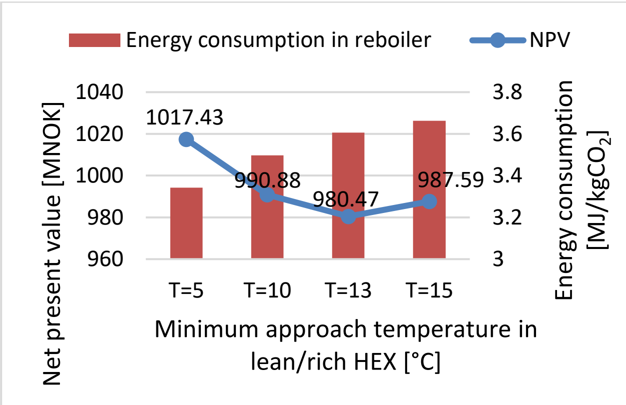

Figure 4. Energy consumption and negative net present value for the minimum approach temperature case.

3.5 85 or 90 % CO_2 removal

Figure 5 shows the specific capture cost (in NOK/ton CO_2 captured) for 85 % and 90 % removal. The cost is distributed on CAPEX, electricity and steam. The figure shows that the steam cost is dominating. 85 % removal gives the minimum specific capture cost. It is however a strategic choice whether 85 or 90 % should be selected because it is not obvious whether a high removal CO_2 or a low specific CO_2 capture cost should be chosen. Compared to more detailed cost estimates on CO_2 capture cost, the calculated cost is probably underestimated (Park et al., 2015). In principle, such an optimization could be performed using a minimization procedure in the Aspen HYSYS spreadsheet.

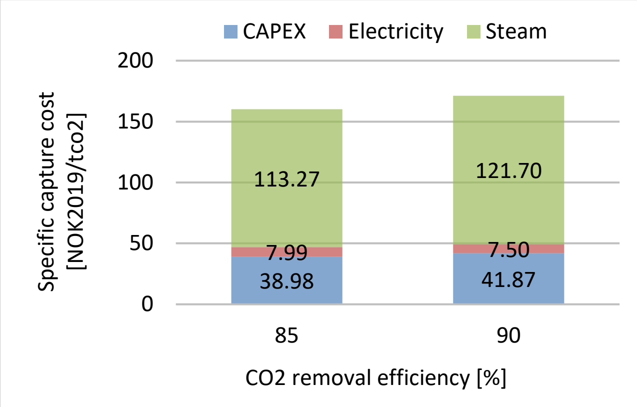

Figure 5. Specific capture cost [NOK/ton CO_2] for 85% and 90 % CO_2 capture.

4 Conclusion

Aspen HYSYS simulations of a standard amine based process for CO_2 capture using an equilibrium based model have been performed in Aspen HYSYS version 10.0 using flue gas data from a cement plant.

The capital cost of CO_2 capture was estimated using equipment cost data from Aspen In-plant and then using a detailed factor method. The cost analysis was limited to the absorption and circulation system, and CO_2 compression or liquefaction was not included. Operating cost was estimated from calculated electricity and heat consumption, and maintenance cost was based on estimated capital cost. Parameters varied were the minimum temperature difference in the main heat exchanger, the number of absorption stages and % CO_2 removed in the process.

Optimum temperature difference in the main heat exchanger was calculated to 10-15 °C, dependent on the specifications. This was found after one simulation for each temperature. Optimum column height was calculated with 12 stages (equivalent to 12 meter of structured packing) based on one simulation for each stage number. Compared to more detailed cost estimates on CO_2 capture cost, the calculated cost of 180-190 NOK (18-19 Euro) is probably underestimated. The scope of the cost calculation is limited to the absorption and circulation system which is most important for parameter optimization.

To obtain really automated calculations it is recommended to improve the robustness of the simulations. This may be achieved by making the material balances more accurate. It should in principle be possible to optimize e.g. the temperature difference in only one automated calculation. To optimize the height (number of stages) in the absorption column automatically, a way to update the number of stages during the simulations has to be found.

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