

Automated Cost Optimization of CO₂ Capture Using Aspen HYSYS

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Abstract

CO₂ can be captured by absorption into monoethanol amine (MEA) followed by desorption. In this work, three configurations; standard, vapour recompression and a simple split-stream (rich split) have been simulated with an equilibrium-based model in Aspen HYSYS™ V10.0 using flue gas data from a natural gas based power plant. Adjust and recycle blocks available in Aspen HYSYS are used to automate the energy and material balance for a specified configuration. Optimization can be performed by minimizing the total cost calculated in an Aspen HYSYS spreadsheet. The equipment cost was obtained from Aspen In-plant Cost Estimator™ V10.0, and an enhanced detailed factor (EDF) method was used to estimate the total investment cost. Parametric studies of absorber packing height, minimum approach temperature in the main heat exchanger, flash pressure and split ratio were performed at 85 % capture efficiency for the three configurations. The calculated cost optimum process parameters for the standard process were 15 m packing height and 13 °C minimum approach temperature. For the vapor recompression case, a flash pressure of 150 kPa provided the lowest total cost. The calculated optimum rich split ratio was 12 %. Automated calculations are dependent on stable convergence of the simulations. A specific challenge is the adjustment of the amine recirculation to obtain a specified total capture rate.

Keywords: Carbon capture, Aspen HYSYS, simulation, cost estimation, optimization

1 Introduction

1.1 Aim

The aim of this work has been to calculate cost optimum process parameters for a standard CO₂ capture process based on amines, with emphasis on the possibility to automate the calculations. Optimization of different configurations, especially vapour recompression and a split stream (rich split) are also evaluated. Such optimizations have been only scarcely documented in literature, and especially a cost optimization of the split-stream ratio has not been found in earlier work.

1.2 Literature

This work is a continuation of previous work at the Telemark University College and the University of South-Eastern Norway (USN). Some references are (Kallevik, 2010; Øi, 2012; Park and Øi, 2017; Aromada and Øi, 2017; Øi et al., 2020). This work is based on the Master thesis work of Haukås (2020).

Several of these projects have involved process simulation, dimensioning and cost estimation of CO₂ capture using the process simulation tool Aspen HYSYS. Capture rate, energy demand and capture cost per ton CO₂ have been calculated.

By changing process parameters, such as the minimum temperature difference in the main heat exchanger, an optimum solution can be found. To keep the specified conditions stable under optimization, different strategies to adjust the process have been used. A traditional challenge is to make sure that the recirculation stream to the amine absorber is the same as in previous iterations. A recycle block available in the simulation program is traditionally used to obtain this. The next challenge is to keep the capture rate constant during iterations. This can be done by adjusting the amine circulation flow to achieve the desired capture rate, either manually or with an adjust block.

1.3 Simulation of process configurations

There have been suggested a number of process improvements of the standard CO₂ capture process (Cousins, 2011a; Moullec et al., 2011; Dubois and Thomas, 2017). Vapour recompression is an alternative where the regenerated amine is pressure reduced, and then the flashed gas is recompressed in a compressor and used as stripping steam in the reboiler. Cost optimization of vapour recompression has been performed by Fernandez et al (2012), Øi et al. (2014), Aromada and Øi (2017) and Øi et al. (2017).

Optimum conditions for a rich split have been evaluated earlier by Cousins et al. (2011b) and Karimi et al. (2011). These publications have emphasis on comparison of energy consumption between different configurations, and on energy optimization by adjusting different parameters for a given configuration.

1.4 Process description

Figure 1 shows a standard process for CO₂ absorption followed by desorption. The equipment units in the flowsheet are an absorption column, a stripping column including a reboiler and condenser, circulating pumps and heat exchangers. The process is described in more detail in Øi (2012), and in Haukås (2020).

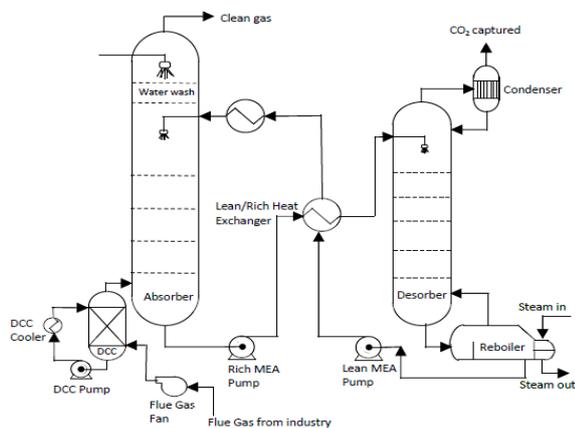


Figure 1. Process flow diagram of a standard amine-based CO₂ capture process (Aromada et al., 2020)

2 Specifications and simulations

2.1 Specifications and simulation of standard CO₂ capture process

The specifications for the base case in Table 1 correspond to 85 % CO₂ removal efficiency and a minimum approach temperature of 10 °C in the lean/rich heat exchanger. The process simulation tool Aspen HYSYS version 10 was used with the amine package (which has now been replaced as the recommended equilibrium model by Aspen HYSYS).

The calculation sequence is similar to earlier works (Aromada and Øi, 2015; Øi et al., 2020). The calculation strategy is based on a sequential modular approach (Kisala et al., 1987; Ishii and Otto, 2008).

Prior to the CO₂ capture process, the flue gas is cooled in a direct contact cooler (DCC) with circulating water. Then the absorption column is calculated from the inlet gas and the lean amine (which is specified in the first iteration). The amine with absorbed CO₂ from the bottom of the absorption column is pumped through the rich/lean heat exchanger with the temperature after the heat exchanger specified. The hot amine solution is entering the desorption column which separates the feed into the CO₂ product at the top and hot regenerated amine at the bottom. The regenerated amine is pumped to a higher pressure in a pump, then passes through the lean/rich heat exchanger and is further cooled in the lean cooler. After the lean amine cooler, the amine solution is checked in a recycle block whether the flow and

composition is sufficiently close to the amine stream from the last iteration.

There are two adjust operations in the flowsheet to get an automated simulation model. One is adjusting the minimum approach temperature in the lean/rich heat exchanger by varying the temperature on the hot side after the exchanger. The other is adjusting the removal efficiency by varying the lean amine mass flow. The Aspen HYSYS process flowsheet is shown in Figure 2.

The traditional process converged after some trial and error. Due to a small water loss (and in some case water build-up) in the process, water must be added to the process. The make-up water was in some simulations adjusted manually and in some calculations the make-up water was calculated by a material balance.

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

Parameter	
Inlet flue gas temperature [°C]	40.0
Inlet flue gas pressure [kPa]	101/121
Inlet flue gas flow rate [kmol/h]	85540
CO ₂ content in inlet gas [mole %]	3.73
Water content in inlet gas [mole %]	6.71
Lean amine temperature [°C]	40.0
Lean amine pressure [kPa]	101.0
Lean amine rate [kg/h]	1.103·10 ⁶
MEA content in lean amine [mass %]	29.0
CO ₂ content in lean amine [mass %]	5.4
Number of stages in absorber [-]	15
Murphree efficiency in absorber [m ⁻¹]	0.15
Rich amine pump pressure [kPa]	500.0
Rich amine temp. out of HEX [°C]	103.6
Number of stages in desorber [-]	12
Murphree efficiency in desorber [m ⁻¹]	0.5
Reflux ratio in stripper [-]	0.4
Reboiler temperature [°C]	120.0
Lean amine pump pressure [kPa]	500.0

2.2 Specification of vapour recompression and split stream processes

The Aspen HYSYS flowsheet for the vapour recompression process is presented in Figure 3. After the desorber, the bottom stream is depressurized through a valve to a flash tank. The gas after the flash tank with a specified flash pressure is compressed and sent back to the desorber. The advantage with the vapour recompression configuration is that the CO₂ content in regenerated amine can be reduced. The drawback is capital and operating cost due to the compressor. Extra specifications are given in Table 2.

Table 2. Aspen HYSYS model parameters and specifications for the vapour recompression case

Parameter	
Flash pressure [bar]	1.0
Compressor outlet pressure[bar]	2.0
Lean pump, delta P [bar]	6.0
Lean MEA flow rate [kmol/h]	92885
CO ₂ content in lean amine [mass %]	5.04
Water content in lean amine [mass %]	68.85
MEA content in lean amine [mass %]	29.11

The Aspen HYSYS flowsheet for the split-stream (rich split) alternative is shown in Figure 4. After the absorption column and the rich MEA pump, the rich amine is split into two streams. One is sent to the top of the desorber while the other stream goes through the main heat exchanger before entering the desorber at a lower feed point. The advantage is that the energy consumption is reduced (Cousins, 2011b). The disadvantage is increased complexity.

2.3 Parameter variations

10 stages, 85 % removal efficiency and 10 °C as minimum approach temperature were specified in the base case simulation. For all the configurations, the packing height and minimum approach temperature were varied. For the vapour recompression case, the flash pressure was varied. For the split-stream case, the split ratio was varied. In the parameter variation simulations, all other specified parameters were kept constant.

When a parameter is varied, the traditional way in a process simulation program like Aspen HYSYS, is to change the parameter to a new value and perform the simulation once more. In many cases it is necessary to perform some adjustments in the flow-sheet to obtain a converged solution. Another possibility is to make use of the Case study function in Aspen HYSYS. In that case a series of calculations can be performed automatically. When using the Case study function, it is not possible to perform other adjustments for each new parameter value.

2.4 Process convergence

The calculation strategy in this work is sequential, even though the Aspen HYSYS simulation tool is in principle equation based. Recycle blocks are used to solve the flowsheet in Aspen HYSYS. Recycle blocks compare the in-stream to the block with the stream from the previous iteration. Adjust functions are used to vary a parameter to obtain a specified result elsewhere in the simulated process. Different tolerances were used in the

recycle blocks and adjust functions to obtain stable and fast convergence. In the columns, the Modified Hysim Inside-Out algorithm with adaptive damping was used according to a recommendation by Øi (2012).

Flow-sheet convergence was discussed by Kisala et al. (1987), Ishii and Otto (2008), Holoboff (2019) and Øi et al. (2020).

As indicated in the subsection about parameter variation, the need for stable convergence is especially important when running a Case study in Aspen HYSYS.

2.5 Simulation and cost estimation procedure

The following procedure was implemented for the cost estimation, similar to the procedure in Øi et al. (2020):

1. Simulation of the CO₂ capture process in Aspen HYSYS with specifications in Table 1 and 2
2. Dimensioning of the equipment
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 (Ali, 2019)
5. Correction for currency and index
6. Estimation of annual operational costs based on energy requirement from simulations
7. Calculation of net present value based on a given discount rate and project lifetime

2.6 Dimensioning and cost estimation

To determine the packing height, a constant stage (Murphree) efficiency corresponding to 1 meter of packing was assumed. Murphree efficiencies of 0.15 and 0.5 were specified for the absorber and the desorber (in Table 1). For the absorber and desorber internals, a structured packing was selected.

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) and Øi et al. (2020). 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.

Centrifugal pumps with 75 % adiabatic efficiency were used in the process simulations.

The direct contact cooler and the flash tank were dimensioned using a Souders Brown equation with k-parameter 0.15 and 0.075 respectively (Souders and Brown, 1934; GPSA, 1987). Overall heat transfer coefficient values have been specified for the lean/rich heat exchanger 550 W/(m²K), lean amine cooler 800 W/(m²K), reboiler 1200 W/(m²K) and condenser 1000 W/(m²K). These values are the same as in Øi (2012) and Park and Øi (2017) and less than the numbers in Øi et al. (2020) which are regarded as optimistic.

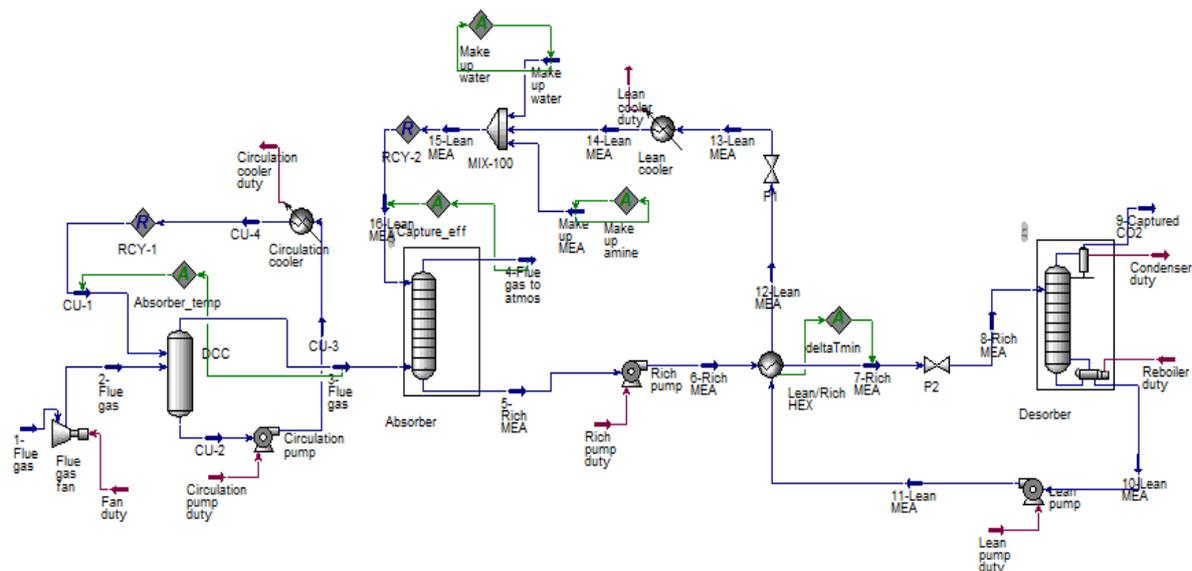


Figure 2. Aspen HYSYS flow-sheet of the base case simulation

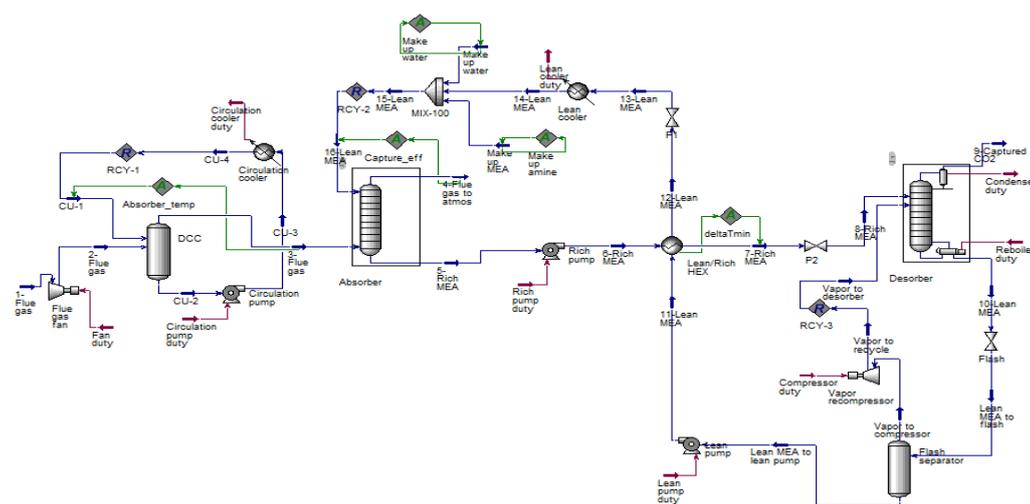


Figure 3. Aspen HYSYS flow-sheet of the vapour recompression case simulation

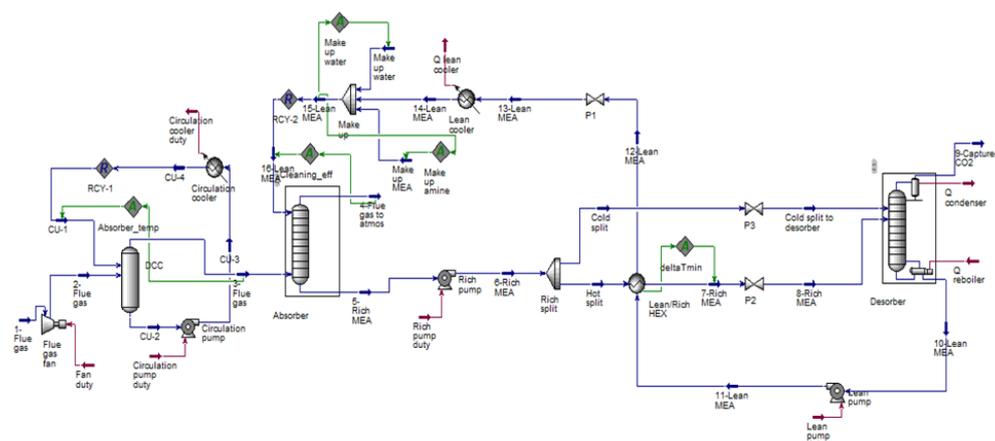


Figure 4. Aspen HYSYS flow-sheet of the split stream simulation

2.7 Capital cost estimation methods

The equipment costs were calculated in Aspen In-plant Cost Estimator (v.10), which gives the cost in Euro (€) for Year 2016 (1st Quarter). A generic location (e.g. Rotterdam) was assumed. Stainless steel (SS316) with a material factor of 1.75 was assumed for all equipment units. For pumps, fan and compressor, a material factor of 1.3 was used as in Øi et al. (2020).

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 Øi et al. (2020). 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 2016 (Eldrup, 2016) were used. More details can be found in Haukås (2020) and Øi et al. (2020).

Table 3. Cost calculation specifications

Parameter	Value
Plant lifetime	20 years
Discount rate	7.5 %
Maintenance cost	4 % 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	9.21
Cost index 2016	103.6
Cost index September 2020	111.3

2.8 Operating cost calculation

This project includes OPEX estimations for the use of electricity and steam. 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, 0.13 NOK/kWh.

2.9 Aspen HYSYS optimization

The spreadsheet unit in Aspen HYSYS was used to calculate the detailed cost estimation of CAPEX, OPEX and NPV (net present value).

For the case of optimizing the temperature difference in the main heat exchanger, the calculation could be performed effectively by using the Case Study option in Aspen HYSYS.

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 flash pressure was optimized by running a series of calculations with different pressures. This was performed both as an Aspen HYSYS Case study and by independent calculations. The split-stream process was also optimized both by a Case study in Aspen HYSYS and with a series of individual calculations.

3 Results and Discussion

3.1 Base case cost results

In Table 4, the results for the capital cost estimation of the base case is given for all the equipment units. The cost is given partly in Euro and partly in NOK, because the Aspen In-plant gives the results in Euro, while the detailed factor method is based on NOK. In the figures 5 to 12 a conversion rate of 10.0 was used to obtain approximate numbers in Euro. At the end of 2020, the conversion rate was exceeding 10.0 (10.2). For the base case, the CAPEX was estimated to 1.3 billion NOK or 130 million Euro.

Table 4. Base case cost results.

Equipment	Eq. cost CS [kEUR2016]	Eq. cost CS [kNOK2016]	Total cost factor CS	Piping factor	Total cost factor SS	Inst. cost [kNOK2020]	Number of units	Installed cost [kNOK2020]
Flue gas fan	5951	55291	3.59	0.29	3.98	236234	-	236234
DCC tower	1985	18443	3.59	0.29	4.56	90299	-	90299
DCC packing*	867	8058	-	-	2.00	17314	-	17314
DCC circ. pump	475	4417	4.93	0.48	5.37	25497	-	25497
DCC circ. cooler	125	1158	6.10	0.65	7.34	9126	6	54754
Absorber shell	2432	22596	3.59	0.29	4.56	110633	-	110633
Absorber packing*	9980	92724	-	-	2.00	199232	-	199232
Water wash*	3327	30911	-	-	2.00	66417	-	66417
Rich pump	174	1612	6.10	0.65	6.60	11417	-	11417
Lean/rich HEX	133	1233	6.10	0.65	7.34	9732	28	272499
Desorber, shell	508	4716	4.44	0.41	5.50	27855	-	27855
Desorber, packing*	1318	12243	-	-	2.00	26307	-	26307
Condenser	56	520	7.20	0.83	8.57	4778	1	4778
Reboiler	128	1188	6.10	0.65	7.34	9416	17	160073
Lean pump	181	1679	6.10	0.65	6.60	11890	-	11890
Lean cooler	100	929	7.20	0.83	8.57	8539	2	17077
Total installed cost								1332277

*Cost estimated in SS 316 in Aspen In-Plant Cost Estimator

3.2 Optimization of column height

The result from the base case is given in Figure 5. It shows an optimum (lowest NPV) for 15 stages equivalent to 15 meter packing height. This is similar to results in earlier work (Kallevik, 2010; Øi et al., 2014; Aromada and Øi, 2017).

Optimum height is also shown for the vapour recompression configuration and the split-stream configuration. Because the change in number of stages has to be performed manually, all the points on the curves in Figures 5, 6 and 7 are performed individually.

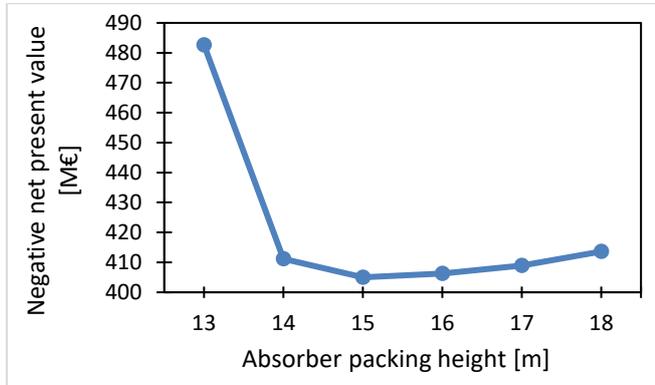


Figure 5. Optimization of number of stages for the standard case.

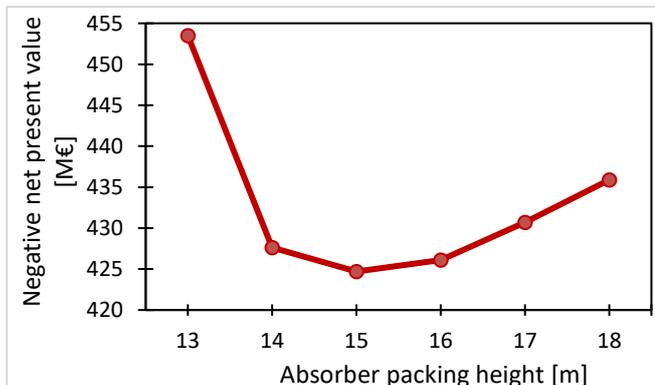


Figure 6. Optimization of number of stages for the Vapour Recompression case

An optimum column height for the vapour recompression case close to the standard process was also found in Øi et al. (2014) and in Aromada and Øi (2017).

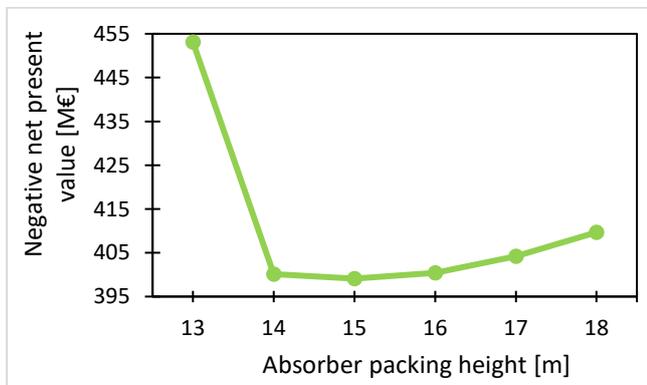


Figure 7. Optimization of number of stages for the Split-Stream configuration

3.3 Optimization of flash pressure

The flash pressure is optimized by a series of calculations. The lowest NPV is at 150 kPa in Figure 8. In this optimization, the column height was 15 meter, and the minimum temperature approach was 10 K. A possible optimum might be found between 150 and 200 kPa, but in that case the extra compressor is not reasonable. The standard process will then be regarded as optimum.

The optimum is sensitive to the cost of the compressor. An optimization was performed with a lower-cost compressor. Then, the cost optimum flash pressure was calculated to 120 kPa. This is closer to other optimization calculations (Øi et al., 2014).

The energy optimum has been calculated to a lower value than the cost optimum by Karimi et al. (2011), Fernandez et al. (2012) and Øi et al. (2014).

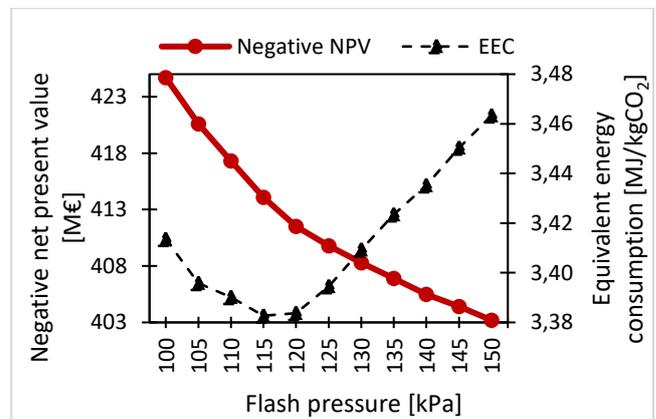


Figure 8. Optimization of flash pressure

3.4 Optimization of split ratio

The optimization in Figure 9 was performed by a Case study in Aspen HYSYS. It shows that the curve is very smooth, and this makes the optimization efficient. The calculated optimum is shown to be 12 %.

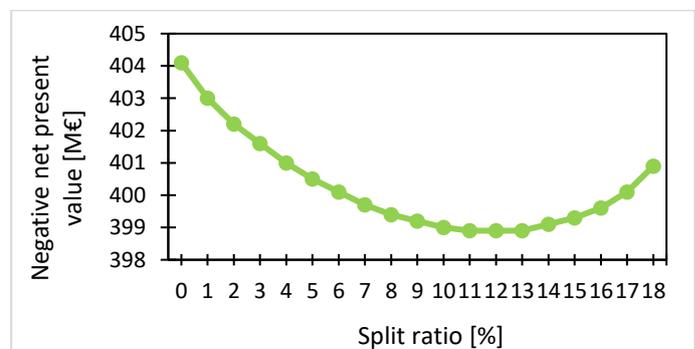


Figure 9. Optimization of the split ratio in a split-stream configuration based on a Case study.

The curve in Figure 9 is very smooth. When the same optimization was performed by manual variation and adjustment of the simulations, the curve was less smooth.

The optimum split ratio was calculated for different specifications. In the optimization in Figure 9, the column height was 15 meter, and the minimum temperature approach was 10 K and optimum lean amine pressure was 500 kPa. The optimum split ratio was calculated to values between 10 and 16 % when these parameters were varied. The optimum capture cost was approximately 40 Euro per ton CO₂ captured in these optimizations. The lowest calculated cost of 39 Euro per ton CO₂ captured was obtained when the pressure increase in the rich amine pump was reduced to 79 kPa.

3.5 Optimum minimum T approach

Minimum temperature approach optimization for the standard, vapour recompression and split-stream configurations are shown in Figure 10, 11 and 12, respectively. The absorber packing height was 15 m in these optimizations. The optimum value can be found as the one with minimum (negative) NPV. The resulting optimum values are 13, 12 and 9 K for three cases. Also, Øi et al. (2014) and Aromada and Øi (2017) get about the same optimum for the different configurations. The optimum minimum temperature approach differs in literature between 10 and 15 K. This is due to different ratios between cost of heat exchangers and cost of heat. All the curves in these three figures are performed by Case studies in Aspen HYSYS. This means that the convergence is rather stable.

Another possibility to optimize is to add a minimization procedure in a spreadsheet connected to the process simulation program. The Aspen HYSYS spreadsheet do not have this as a function. But one possibility is to link the Aspen HYSYS simulation to another tool like an Excel spreadsheet. This is discussed by Sharma and Rangaiah (2016).

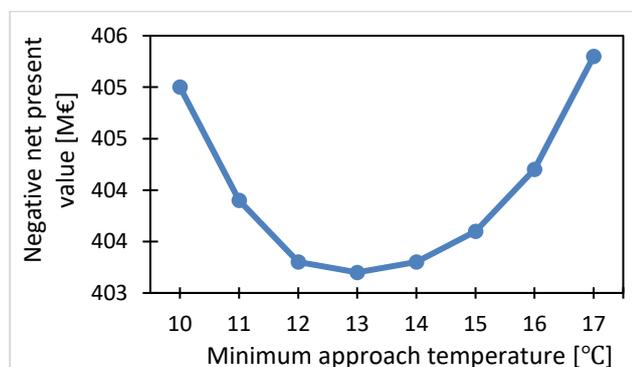


Figure 10. Optimization of minimum approach temperature for the base case

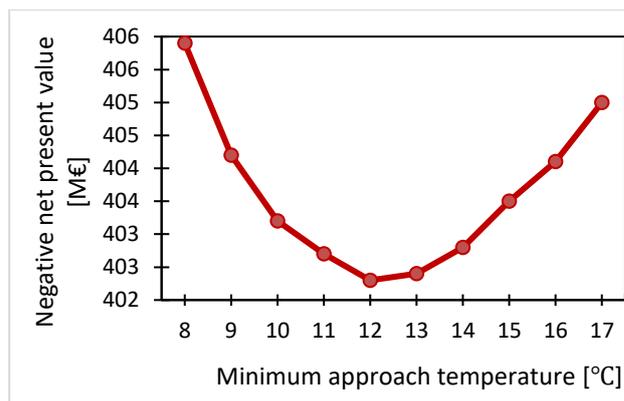


Figure 11. Optimization of minimum approach temperature for the vapour recompression case.

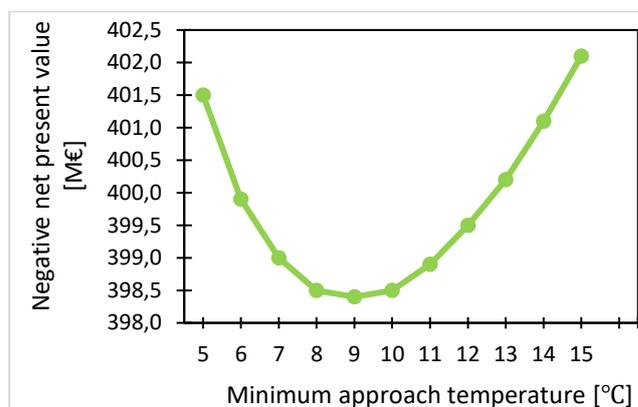


Figure 12. Optimization of minimum approach temperature for the split-stream case.

The optimum capture cost was calculated to approximately 40 Euro per ton CO₂ captured in these optimizations. This is in order of magnitude the last year's quota price for CO₂. When cost of transport and storage is added, the cost of capture, transport and storage is still higher than the quota price.

4 Conclusion

In this work, three configurations; standard, vapour recompression and a simple split-stream (rich split) have been simulated with an equilibrium-based model in Aspen HYSYS™ using flue gas data from a natural gas based power plant. Adjust and recycle blocks available in Aspen HYSYS are used to automate the energy and material balance for a specified configuration. Optimization can be performed by minimizing the total cost calculated in an Aspen HYSYS spreadsheet. The equipment cost was obtained from Aspen In-plant Cost Estimator™ V10.0, and an enhanced detailed factor (EDF) method was used to estimate the total investment cost. Parametric studies of varying absorber packing height, minimum approach temperature, flash pressure and split ratio were performed at 85 % capture efficiency for the three configurations. The calculated

cost optimum process parameters for the standard process were 15 m packing height and 13 °C minimum approach temperature. For the vapour recompression case, a flash pressure of 150 kPa provided the lowest total cost. The calculated optimum for the rich split configuration was 10-16 % split ratio. The minimum capture cost was calculated to 39-40 Euro per ton CO₂ in these optimizations. Automated calculations are dependent on stable convergence of the simulations. A specific challenge is the adjustment of the amine recirculation to obtain a specified total capture rate.

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