Process Simulation and Cost Optimization of CO_2 Capture Configurations in Aspen HYSYS

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Abstract

A CO_2 capture process from a natural gas based power plant has been simulated and cost estimated using an equilibrium-based model in Aspen HYSYS using the amine acid gas package. The aim has been to calculate cost optimum process parameters for the standard process and also for a vapor recompression process. After process simulation using Aspen HYSYS, the process equipment was dimensioned and cost estimated using Aspen In-plant. The Enhanced Detailed Factor (EDF) method was used to select factors to calculate the total investment. Operating cost for heat and electricity was calculated from the simulation with estimated cost on consumed heat and electricity. The cost was calculated to 21.2 EURO per ton CO_2 removed and a vapor recompression process was calculated to 21.6 EURO per ton. A recompression case with 1.2 bar flash pressure was calculated to 21.3 EURO/ton CO_2. The ΔT_{MIN} in the amine/amine heat exchanger was varied, and the optimum at 15°C was 20.9 EURO per ton CO_2. The vapor recompression alternative was in this work slightly more expensive than the traditional case. In earlier works, the vapor recompression process has been claimed to be more economical than the standard process. The difference in this work is mainly due to different cost estimates of the compressor investment. This work shows that Aspen HYSYS is well suited for optimizing process parameters in a CO_2 capture process with and without vapor recompression.

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

1. Introduction

CO_2 capture based on absorption into an amine followed by desorption is an established method to reduce CO_2 emissions. Much work has been performed on simulation and cost estimation of CO_2 capture processes, especially from natural gas based power plants. A traditional tool has been an equilibrium-based model in Aspen HYSYS using the amine acid gas package. The aim has often been to calculate cost optimum process parameters for a standard process. In this work, the main aim has been to calculate cost optimum process parameters for a standard CO_2 capture process. A special aim has been to compare the standard process with a process based on vapor recompression. It shows that it is difficult to state whether the vapor recompression process is more economical than a standard CO_2 capture process.

2. Literature, Process Description and Specifications

2.1 Literature

There are several papers presenting results from process simulation and cost estimation of CO_2 capture plants (Manzolini et al., 2015; Luo and Wang, 2016; Nwaoha et al., 2018; Hasan et al., 2021). 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; Aromada and Øi, 2017; Øi et al., 2020; Øi et al., 2021; Shirdel et al. (2022). These projects have involved process simulation, dimensioning and cost estimation of CO_2 capture using the process simulation tool Aspen HYSYS. Capture rate, energy demand and capture cost per ton CO_2 have been calculated. Many of the projects have optimized parameters by changing one process parameter at a time, such as the minimum temperature difference in the main heat exchanger.

In the literature there have been presented many suggestions for process improvements using different process configurations (Cousins et al., 2011; Moullec et al., 2011; Dubois and Thomas, 2017). A simple alternative is vapor recompression where regenerated amine is depressurized into a flash tank, and the flash gas is recompressed and sent to the bottom of the desorber. Cost optimization of vapor recompression has been perfomed by Fernandez et al. (2012), Øi et al. (2014), Aromada and Øi (2017), Øi et al. (2017) and Øi et al. (2021). This work is based on a Master group project (Kermani et al., 2022). In addition to the project work, simulation and cost estimation of the vapor compression process from 1.2 to 2 bar was also included.

2.1. Process description of a standard process

Fig. 1 shows a typical process for CO_2 capture using an amine absorbent. In this method, CO_2 is absorbed and captured in an aqueous amine solution, in which flue gas is passed through. The CO_2-rich amine is then sent to a stripper, is heated with steam, and as a result CO_2 is released from the solution. In the figure, a gas cooler before the absorber and a water wash are shown, but these units are not simulated in this work.

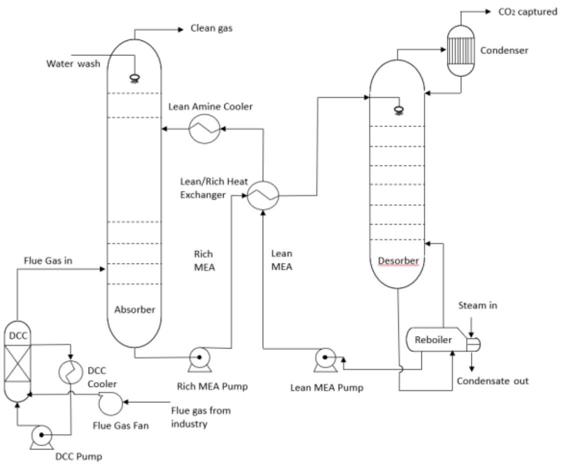

Figure 1: Process flow diagram of a standard amine-based CO_2 capture process (Aromada et al., 2020)

3 Specifications and simulations

3.1 Specifications and simulation of standard CO_2 capture process

The specifications for the base case is given in Table 1. The calculation sequence is similar to earlier works (Aromada and Øi, 2015; Øi et al., 2020; Øi et al, 2021). The absorption column is calculated first based on the inlet gas and the estimated lean amine flow (which is specified in the first iteration). The amine from the bottom of the absorption column is sent to regeneration via the rich/lean heat exchanger. The amine flow is entering the desorption column which separates the feed into CO_2 product at the top and hot regenerated amine at the bottom. The regenerated amine is returned via the lean/rich heat exchanger and the lean cooler to the recycle block. Due to water loss in the process, water must be added to the process. The make-up water was adjusted manually. The specifications in Table 1 aim at a 90 % CO_2 removal efficiency and gives the result of 7.7 °C in the lean/rich heat exchanger. The simulations were performed in Aspen Plus V12.

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]	110
Inlet flue gas flow rate [kmol/h]	85000
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]	110.0
Lean amine rate [kg/h]	110000
MEA content in lean amine [mol-%]	11.21
CO_2 content in lean amine [mol-%]	2.93
Number of stages in absorber [-]	10
Murphree efficiency in absorber [m^{-1}]	0.25
Rich amine pump pressure [kPa]	200.0
Rich amine temp. out of HEX [°C]	104.9
Number of stages in desorber [-]	6
Murphree efficiency in desorber [m^{-1}]	1
Reflux ratio in stripper [-]	0.3
Reboiler temperature [°C]	120.0
Lean amine pump pressure [kPa]	500.0

3.2 Specification of vapor recompression process

The Aspen HYSYS flowsheet for the base case is presented in Fig. 2. The flowsheet for the vapor recompression process is presented in Fig. 3. After the desorber, the amine is pressure reduced through a valve to a flash tank. The gas after the flash tank with atmospheric pressure (or higher) is compressed and sent back to the desorber. Except for this, the process is the same as in the base case.

3.3 Parameter variations

With a 110000 kg/h amine flowrate, absorption 10 stages, 90 % removal efficiency and 7.7 °C minimum approach temperature were obtained in the base case simulation. The minimum approach temperature was varied. For the vapor recompression case, the flash pressure was varied. In the parameter variation simulations, all other specified parameters were kept constant.

A possibility is to make use of the Case study function in Aspen HYSYS. In that case a series of calculations can be performed automatically keeping all other specified parameters constant.

3.4 Simulation and cost estimation procedure

The objective of this part is the estimation of the plant's total cost for the designed CO_2 capture process. Calculations are based on dimensions obtained from the simulation in Aspen HYSYS V12. A short version of the cost estimation procedure is as follows, similar to the procedure in Øi et al. (2020) and Øi et al. (2021):

- Calculation of each equipment cost using Aspen In-Plant Cost Estimator, based on equipment dimensioning parameters for the base case.
- Calculation of the total installation cost by applying the Enhanced Detailed Factor (EDF) method.
- Correction of total installation cost by the cost inflation index (conversion by year).
- Calculation of annualized capital expenditure (CAPEX) according to the discount rate and lifetime
- Calculation of annual operational expenditure (OPEX)
- Calculation of the total CO_2 capture cost based on the plant lifetime

3.5 Dimensioning for cost estimation

The estimation of packing height is based on a constant stage (Murphree) efficiency corresponding to 1 meter of packing. Murphree efficiencies were specified to 0.25 for the absorber and 1.0 for the desorber. Structured packing was assumed.
The estimation of absorption column diameter was based on a gas velocity of 2.5 m/s and for the desorption column a gas velocity of 1 m/s was assumed as in Øi et al. (2020) and Øi et al. (2021). The total height of the absorption column and desorption column were specified to be 25 m and 16 m respectively. The extra height is due to distributors, water wash packing, demister, gas inlet, outlet and sump. The pumps and the vapor compressor were specified to have 75 % adiabatic efficiency.
Overall heat transfer coefficient values were specified for the lean/rich heat exchanger 500 W/(m^{2}K), lean amine cooler 800 W/(m^{2}K), reboiler 1200 W/(m^{2}K) and condenser 1000 W/(m^{2}K). These values are the same as in Øi et al. (2021) except for the lean/rich heat exchanger number (changed from 550 W/m^{2}K), and slightly less than the numbers in Øi et al. (2020).

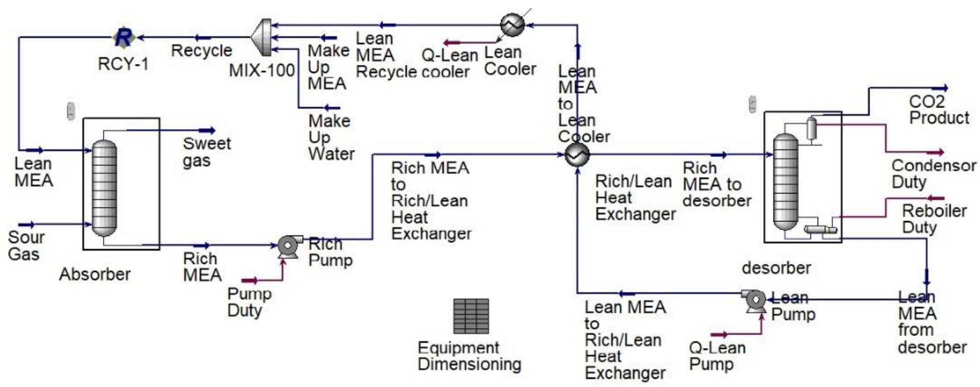

Figure 2. Aspen HYSYS flow-sheet of the base case simulation (from Kermani et al., 2022)

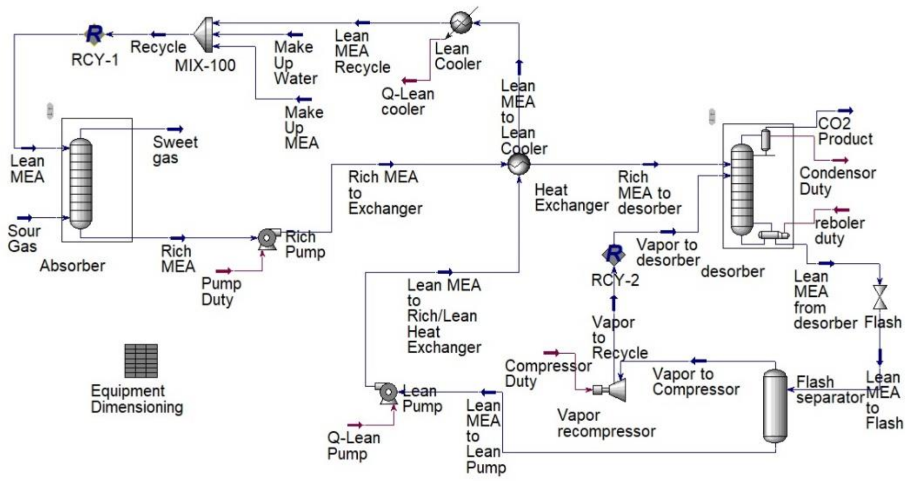

Figure 3. Aspen HYSYS flow-sheet of the vapour recompression case simulation (from Kermani et al., 2022)

3.6 Capital cost estimation methods

Equipment costs were calculated in Aspen In-plant Cost Estimator (version 12), which gives the cost in Euro (€) for Year 2016 (1st Quarter). Stainless steel (SS316) with a material factor of 1.75 was assumed for all equipment units, except for pumps and the vapor compressor where a material factor of 1.3 was used as in Øi et al. (2020) and Øi et al (2021).

In the EDF detailed factor method, each equipment cost in carbon steel was multiplied with an installation factor to obtain installed cost. 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. Installation factors from Aromada et al. (2021) were used.

Table 3. Cost calculation specifications

Parameter	Value
Plant lifetime	10 and 20 years
Discount rate	7.5 %
Maintenance cost	4 % of installed cost
Electricity price	0.06 EURO/kWh
Steam price	0.015 EURO/kWh
Annual operational time	8000 hours
Location	Rotterdam

3.7 Operating cost calculation

This project includes OPEX estimations for the use of electricity and steam (maintenance cost is not included). Operating cost specifications are given in Table 3. Electricity cost was specified to be 0.06 EURO/kWh (approximately 0.6 NOK/kWh). The steam cost was specified to be 25 % of the electricity cost, 0.015 EURO/kWh. This is reasonable for a case where the heat could be converted to electricity with 25 % efficiency. The detailed cost estimation of CAPEX, OPEX and NPV (net present value) were calculated in an internal spreadsheet in Aspen HYSYS.

4 Results and Discussion

4.1 Base case cost results

In Fig. 4, the results for the capital cost estimation of the base case are shown for all the equipment units. The total cost was calculated to 74.6 mill. EURO. The total cost per ton CO_2 removed was calculated to 21.2 EURO/ton CO_2. The numbers are low compared to many other estimations, but the values in Øi et al. (2020) are similar. One reason is that some equipment like pre-treatment and water wash is not included in these calculations. However, for optimization calculations, only the units in the recirculation are necessary to obtain a reasonable optimization.

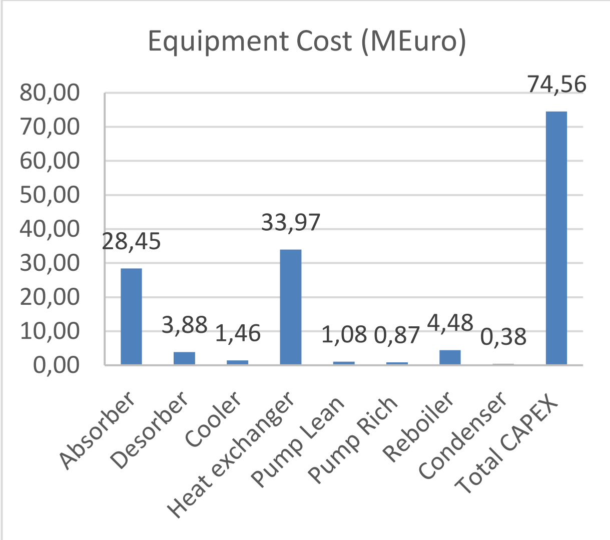

Figure 4: Total CAPEX and the cost of each piece of equipment for the base case (Kermani et al., 2022).

The equipment cost shows that the most expensive equipment units are the absorber and the main heat exchanger. This is traditional. Normally the absorber is the most expensive unit, so there is a possibility that the absorber cost is underestimated. The estimated column efficiency is 0.25 per meter packing height, which is optimistic compared to 0.15 in Øi et al. (2021). A water wash is normally a part of the absorber, and this cost is neglected in this work. The total cost is probably also underestimated because there are probably equipment unit details that are more complex than assumed. The operating cost is probably underestimated because the maintenance cost is not included. If both CAPEX and OPEX is underestimated to the same degree, the trade-off between them will give reasonable cost optimum parameters.

4.2 Vapour recompression case

The vapor recompression cost was calculated to 21.6 EURO/ton CO_2 for a flash pressure of 1 bar. This is slightly higher than the standard process, and in this work this was not optimum. The cost was also calculated for a flash pressure of 1.2 bar, and the result was 21.3 EURO/ton CO_2. This was the optimum vapour recompression case, but it was still not optimum compared to the base case. In earlier work (Karimi et al., 2011; Øi et al., 2014), the vapour recompression case was estimated to be the most optimum process. The difference in this work is mainly due to different estimates of the compressor investment. It is possible to reduce the cost of the vapor recompression by optimizing the flash pressure as in Fernandez et al. (2012). In Øi et al. (2021), a flash pressure of 1.5 bar was the optimum in the vapour recompression case, but was not better economically than the standard process.

4.3 Optimum minimum temperature approach

The total cost was calculated for different temperature approaches. The result is shown in Fig. 5 with the base case shown for 7.7 K. The absorber packing height was 15 m in these optimizations. The optimum value was found as the one with minimum total cost at 15 K with 20.9 EURO/ton. Øi et al. (2014) and Aromada and Øi (2017) get about the same optimum. Values for the optimum minimum temperature approach in literature are often between 10 and 15 K.

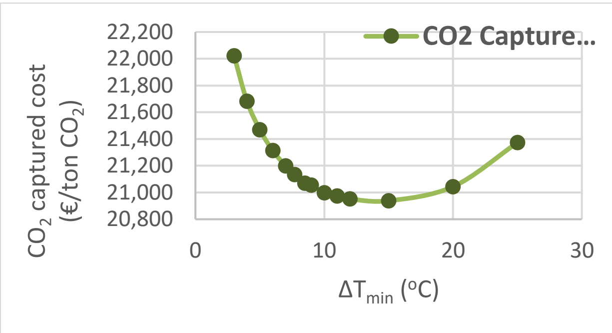

Figure 5. Optimization of minimum approach temperature for the base case (Kermani et al., 2022)

4.4 Comparison with earlier studies

The numbers in Table 4 show different literature sources with typical or optimized values for CO_2 capture rate, inlet CO_2 concentration, ΔT_{min}, absorber packing height and reboiler duty. The table shows that the calculated and estimated temperature approach, reboiler duty and absorber height are similar to values found in literature.

Table 4. Comparison of this study with previous base case scenarios

Study	CO_2 capture rate [%]	CO_2 con. [mol %]	ΔTmin [°C]	Absorber packing height [m]	Reboiler du [kJ/capture CO_2 kg]
Present work (base case)	90	3.73	7.7	10 (25-total height)	3757
Present work (ΔT_{min} =10)	90	3.73	10	10	3852
Aromada et al. [11]	85	3.73	10	10	3600
Øi et al. [15]	85	3.75	10	10	3650
Alhajaj et al. [24]	90	5	20	34.3	4484
Amrollahi et al. [25]	90	3.8	8.5	13	3740
Sipöcz et al. [26]	90	4.2	10	26.9 (Total height)	3930
Karimi et al. [9]	90	11.86	5	7	3545
	90	11.86	10	7	3611

Some of the numbers are optimized and some of them are typical or reasonable values. Most of them are for CO_2 capture processes for natural gas based power plants with about 4 mol-% CO_2 in the exhaust gas as in this work. The rounded values in the values shown in Table 4 indicate that there is need for further work to find optimum values for these parameters.

5. Conclusion

A CO_2 capture process from a natural gas based power plant has been simulated and cost estimated using an equilibrium-based model in Aspen HYSYS using the amine acid gas package. The aim has been to calculate cost optimum process parameters for the standard process and also for a vapor recompression process.

After process simulation using Aspen HYSYS, the process equipment was dimensioned and cost estimated using Aspen In-plant. The Enhanced Detailed Factor (EDF) method was used to select factors to calculate the total investment. Operating cost for heat and electricity was calculated from the simulation with estimated cost on consumed heat and electricity. The cost was calculated to 21.2 EURO per ton CO_2 removed and a vapor recompression process was calculated to 21.6 EURO per ton.

The ΔT_{MIN} in the amine/amine heat exchanger was varied, and the optimum at 15°C was 20.9 EURO per ton CO_2. The vapor recompression alternative also calculated with 1.2 bar flash pressure, was in this work slightly more expensive than the traditional case. In earlier works, the vapor recompression process has been claimed to be more economical than the standard process. The difference in this work is mainly due to different cost estimates of the compressor investment.

This work shows that Aspen HYSYS is well suited for optimizing process parameters in a CO_2 capture process with and without vapor recompression.

References

Ali, H. (2019) *Techno-economic analysis of CO_2 capture concepts.* PhD Thesis, University of South-Eastern Norway.

Alhajaj, A. (2016) 'A techno-economic analysis of post-combustion CO_2 capture and compression applied to a combined cycle gas turbine: Part II. Identifying the cost-optimal control and design variables', *International Journal of Greenhouse Gas Control*, 52:331-343, doi: 10.1016/j.ijggc.2016.07.008.

Amrollahi, P. A. M. et al. (2012) 'Optimized process configurations of post-combustion CO_2 capture for natural-gas-fired power plant – Power plant efficiency analysis', *International Journal of Greenhouse Gas Control*, 8:1-11, doi: 10.1016/j.ijggc.2012.01.005.

Aromada, S. A. and Øi, L.E. (2017) 'Energy and economic analysis of improved absorption configurations for CO_2 capture.' *Energy Procedia*, 114: pp. 1342-1351.

Aromada, S. A. et al. (2021) 'Capital cost estimation of CO_2 capture plant using Enhanced Detailed Factor (EDF) method: Installation factors and plant construction characteristic factors', *Int. J. Greenh. Gas Control*, vol. 110, no. 1, p. 103394, doi: 10.1016/j.ijggc.2021.103394.

Cousins A. et al. (2011) 'A survey of process flow sheet modifications for energy efficient CO_2 capture from flue gases using chemical absorption'. *International Journal of Greenhouse Gas Control*, 5(4):605-619.

Dubois, L. and Thomas, D. (2017) 'Comparison of various configurations of the absorption-regeneration process using different solvents for the post-combustion CO_2 capture applied to cement plant flue gases.' *International Journal of Greenhouse Gas Control*, 69:20-35.

Eldrup, N. (2016) *Installation factor sheet - Project Management and Cost Engineering*. Master's Course. University College of South-Eastern Norway, Porsgrunn.

Eldrup, N. et al. (2019) 'A Cost Estimation Tool for CO2 Capture Technologies', SSRN Scholarly paper ID 3366036, doi: 10.2139/ssrn.3366036

Fernandez, E. S. et al. (2012) 'Optimisation of lean vapour compression (LVC) as an option for post-combustion CO_2 capture: Net present value maximisation.' *International Journal of Greenhouse Gas Control*, 11:114-121.

GPSA (1987), *Engineering Data Book, 10. ed., Tulsa, Oklahoma: Gas Processing Suppliers Association, 1987.*

Hasan, S. et al. (2021) 'Improving the Carbon Capture Efficiency for Gas Power Plants through Amine-Based Absorbents', *Sustainability*, 13(1), doi: 10.3390/su13010072

Kallevik, O. B. (2010) *Cost estimation of CO_2 removal in HYSYS*. Master's Thesis, Telemark University College, Porsgrunn.

Karimi, M. et al. (2011) 'Capital costs and energy considerations of different alternative stripper configurations for post combustion CO_2 capture.' *Chemical Engineering Research and Design*, 89(8):1229-1236.

Kermani, S. H. et al. (2022) 'Process simulation and cost estimation of CO_2 capture configurations in Aspen HYSYS.' Master project, University of South-Eastern Norway.

Luo, X and Wang, M. (2016) 'Optimal operation of MEA-based post-combustion carbon capture for natural gas combined cycle power plants under different market conditions," *International Journal of Greenhouse Gas Control*, 48, pp. 312-320. doi: 10.1016/j.ijggc.2015.11.014.

Manzolini, G. et al. (2015) 'Economic assessment of novel amine based CO_2 capture technologies integrated in power plants based on European Benchmarking Task Force methodology'. *Applied Energy*, 138, pp. 546-548

Nwaoha, C. *et al.* (2018), 'Techno-economic analysis of CO_2 capture from a 1.2 million MTPA cement plant using AMP-PZ-MEA blend', *International Journal of Greenhouse Gas Control*, 78 pp. 400-412.

Sipöcz, N. et al. (2011), 'Integrated modelling and simulation of a 400 MW NGCC power plant with CO_2 capture', *Energy Procedia*, 114: pp. 1342-1351.

Shirdel, S. *et al.* 'Sensitivity Analysis and Cost Estimation of a CO_2 Capture Plant in Aspen HYSYS'. *Chem. Engineering*, 6(2), 28, 2022.

Souders, M. and Brown, G. G. (1934) 'Design of Fractionating Columns I. Entrainment and Capacity.' *Industrial & Engineering Chemistry*, 26:98-103.

Øi, L. E. (2012) *Removal of CO_2 from exhaust gas*. PhD Thesis, Telemark University College, Porsgrunn.

Øi, L E. et al. (2014) 'Optimization of Configurations for Amine based CO_2 Absorption Using Aspen HYSYS.' *Energy Procedia*, 51: 224-233.

Øi, L. E. and Sundbø, E. (2017) '*Simulation and Economic Optimization of Vapor Recompression Configuration for Partial CO_2 capture*.' In the 58th Conference on Simulation and Modelling, SIMS 58, Reykjavik, Iceland.

Øi, L. E. *et al. (2021)* 'Automated Cost Optimization of CO_2 Capture Using Aspen HYSYS', Linköping Electronic Conference Proceedings SIMS 62, pp. 293-300. doi: 10.3384/ecp21185293