Process Simulation, Dimensioning and Automated Cost Optimization of CO_2 Capture

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Abstract

A standard process for CO_2 capture has been simulated with an equilibrium-based model in Aspen HYSYS. The simulation has been combined with equipment dimensioning and cost calculation in an integrated spreadsheet facility. New in this work is that Murphree efficiencies are varied to obtain automatic optimization of absorber height and inlet temperature. The optimum process was found as the process with minimum calculated sum of capital and operational cost over 25 years. The cost optimum process parameters for the standard process were calculated to 15 m absorber packing height, 13 K minimum approach temperature and 34 °C in inlet gas temperature. This study demonstrates that it is possible to calculate the optimum packing height and inlet temperature automatically by varying the Murphree efficiency in a case study function.

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

1. Introduction

1.1. Aim

The general aim of this work is to calculate the cost optimum absorption column height, minimum temperature approach temperature in the main amine/amine heat exchanger and optimum inlet temperature to the absorber. A specific aim is to make it possible to calculate these optimums automatically by varying the Murphree efficiency.

1.2. Literature

Much work has been published on cost estimation of CO_2 capture plants (Rubin *et al*., 2013; van der Spek *et al*., 2019; Roussanaly *et al*., 2021). Several papers present results from process simulation and cost estimation (Mores *et al.*, 2012; Agbonghae *et al.*, 2014); Manzolini *et al*., 2015; Luo and Wang, 2016; Nwaoha *et al*., 2018; Eldrup *et al*., 2019; Hasan *et al*., 2021).
Some of the previous works at Telemark University College and the University of South-Eastern Norway (USN) with focus on process simulation, equipment dimensioning, cost estimation and optimization are Kallevik (2010), Øi (2007), Øi (2012), Aromada and Øi (2017) and Øi *et al*. (2022). The cost estimation part has in most of these works been based on different detailed factor methods like the Enhanced Detailed Factor (EDF) method (Ali *et al*., 2019; Aromada *et al*., 2021). In these works, the main approach for calculating the optimum has been to use case studies in Aspen HYSYS and varying only one parameter at a time. Then the optimum is found as the simulation giving the minimum sum of capital and operational cost.
In the recent years, a focus has been on automatic process simulation combined with cost estimation in Aspen HYSYS (Øi *et al*., 2021; Øi *et al*., 2022; Shirdel *et al.*, 2022). An Iterative Detailed Factor (IDF) scheme was developed (Aromada *et al*., 2022a) where an aim was to make the entire process simulation, equipment dimensioning and cost estimation automatic, without requiring any manual input. This was accomplished in the work by Øi *et al*. (2022) by linking Aspen HYSYS simulation spreadsheets with Microsoft Excel by a VBA (Visual Basic) code. With an automated approach, process simulation based CO_2 capture, process parameter cost optimization studies and sensitivity analysis can be conducted quickly and obtain reasonably accurate results.
A limiting factor for automation in the Aspen HYSYS tool, has been that for a column, the number of equilibrium stages must be changed manually. To overcome this, a possibility is to vary the Murphree efficiency on one or a selected number of absorption stages. The optimization can then be performed by performing a case study in Aspen HYSYS. This work is based on the results from the Master thesis work of Shirdel (2022), and in addition more references are included and discussed.

1.3. Process Description

The use of an amine solvent to remove CO_2 is the most widely used and well-studied approach for CO_2 removal. Monoethanol amine (MEA) is the solvent that has been studied most, and it works well due to its quick interaction with CO_2. Fig. 1 is a typical process flow diagram for an amine-based CO_2 removal facility. Traditional absorption is done in a column using plates, random packing or structured packing. The CO_2-containing gas rises, while the absorption liquid falls. The solvent (rich amine) is then fed to a desorption column through a heat exchanger. In the desorption (stripper) column, the CO_2 that has been absorbed is regenerated. The reboiler is heated, and a condenser provides reflux to the column. The regenerated solvent (lean amine) is recirculated to the absorption column after the desorber and cooled in a heat exchanger and cooler.

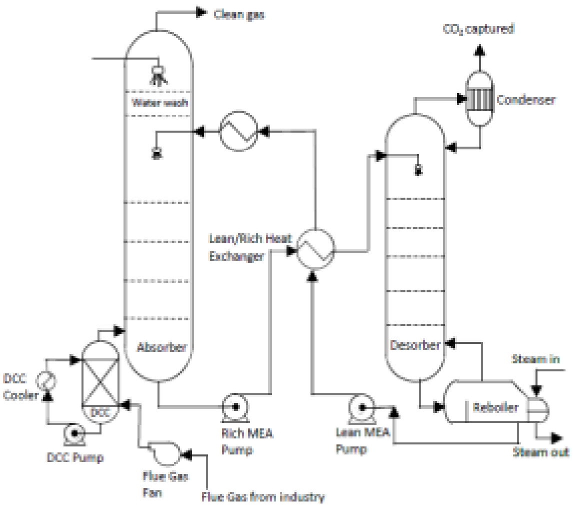

Figure 1: Process flow diagram of a standard amine-based CO_2 capture process (Aromada *et al*., 2020).

2. Specifications and simulations

2.1. Specifications and simulation of base case CO_2 capture process

In this investigation, Aspen HYSYS version 12 was used to model a conventional amine-based CO_2 capture process, and the simulated results were utilized to size equipment and estimate costs using the same calculation method as in Aromada et al. (2021), Øi *et al*. (2021) and Øi *et al*. (2022). In all simulations, the Acid Gas property package was employed, which includes a liquid equilibrium model for electrolytes. This package is intended to replace the Amine property package, which has been widely used when using the Aspen HYSYS tool. The electrolyte non-random two-liquid (e-NRTL) model for electrolyte thermodynamics and the Peng-Robinson equation of state for the vapor phase were used to create this property package.

The absorber and desorber were simulated using equilibrium stages containing user defined stage (Murphree) efficiencies. These Murphree efficiencies are defined by dividing the change in CO_2 mole fraction from one stage to the next by the change on the assumption of equilibrium.

Emission data from previous studies (Aromada and Øi, 2017) on a natural gas-based power plant project on Mongstad, Norway, were utilized to generate the base case for the simulations. The specifications in Table 1 correspond to an 85 per cent CO_2 removal efficiency and a minimum approach temperature of 10 °C in the lean/rich amine heat exchanger, which is considered the base case configuration. 85 % CO_2 removal rate is traditional for capture from power plant based on natural gas. The absorber is modelled with 15 packing stages, while the desorber has 10. Murphree efficiencies of 15% were employed in the absorption column and 50% for all stages of the desorption column where one stage is expected to be approximately 1 meter packing height. In the columns, the Modified HYSIM Inside-Out numerical solver was adopted since it assists in convergence. The adiabatic efficiency of the pump and flue gas fan was specified to be 75%.

To obtain an automated simulation model, robust adjustments and recycles are necessary to aid in the convergence of the simulations. Traditionally, manual adjustments can be performed by trial and error when working with a complex simulation model.

The calculation sequence is similar to the simulations in Øi *et al.* (2021) and Øi *et al.* (2022). It starts with the input gas and the lean amine to the absorption column (which is first guessed). The rich amine pump transports the rich amine from the bottom of the absorption column through the lean/rich amine heat exchanger. After the heat exchanger, the temperature is specified, and the rich amine is sent to the desorber. The CO_2 product and the hot lean amine are calculated in the desorption column. The heated lean amine is passed via the lean/rich heat exchanger and then pressurized in the lean amine pump, before being cooled further in the lean cooler. Water was added to the process (water make-up) and the make-up was calculated by a water material balance.

The lean amine is then placed in a recycle block (RCY_1). It is determined whether the recycled lean amine's flow and condition are sufficiently similar to the previously estimated lean amine stream, which may be adjusted through iteration.

In order to create an automated simulation model, three adjust operations were added to the flowsheet. The removal efficiency can be adjusted based on the lean amine flow rate by ADJ-1, the minimum approach temperature in the lean/rich heat exchanger may be adjusted based on the rich amine outlet temperature of the lean/rich heat exchanger by

ADJ-2, and for adjusting the flue gas temperature to the absorber, ADJ-3 changes the cooling water supply in the inlet cooler. The default tolerances in Aspen HYSYS were used in the simulations.

Table 1: Specifications for the base case alternative

Parameter	**Value**
Inlet flue gas temperature [ºC]	80/40.0
Inlet flue gas pressure [kPa]	101/115
Inlet flue gas flow rate [kmol/h]	85000
CO_2 content in inlet gas [mole %]	3.75
Water content in inlet gas [mole %]	6.71
Lean amine temperature [ºC]	40.0
Lean amine pressure [kPa]	101.0
Lean amine rate [kg/h]	103500
MEA content in lean amine [mass %]	29
CO_2 content in lean amine [mass %]	5.5
Number of stages in absorber [-]	15
Murphree efficiency in absorber	0.15
Rich amine pump pressure [kPa]	200.0
Rich amine temp. out of HEX [ºC]	103.7
Number of stages in desorber [-]	10
Murphree efficiency in desorber	0.5
Reflux ratio in stripper [-]	0.3
Reboiler temperature [ºC]	120.0
Lean amine pump pressure [kPa]	500.0

2.2. Parameter variation of ΔT_{min}

A case study was made to look into the economic performance of the lean/rich amine heat exchanger when the degree of heat recovery was adjusted. More heat recovery will normally increase the capital cost and reduce the operating cost. The ΔT_{min} was changed for each simulation case. This was performed automatically by changing the target temperature from 5 to 20 °C in ADJ-2, whereas the ADJ-1 and ADJ-3 will aim to maintain a constant CO_2 removal efficiency of 85% and a constant incoming flue gas temperature of 40 °C, respectively. All flue gas and absorption column parameters were held constant throughout the case for a certain total CO_2 removal efficiency, lean amine composition and lean amine flow.

2.3. Parameter variation of number of absorption stages and absorber height

A higher absorption column packing is expected to increase the capital cost and reduce the operating cost. Because each change in the number of stages in the Design tab of the absorber requires manual input to run the simulation again, the case study option cannot be utilized in the sensitivity analysis for altering absorber height (stages). In all stages, Murphree efficiency has been set to 0.15. For each case, the efficiency of new stages, the pressure of flue gas into the absorber, and the pressure in the absorber's last stage should all be updated. For this reason, a new spreadsheet was created, and the calculations for changing the number of stages of the absorber and fan outlet pressures based on 1 kP for each stage (Park and Øi, 2017) were performed.

In this study, a strategy was employed to define a case study by altering the efficiency of one specific stage. Changing the efficiency at one stage from 0.15 to 0.9 for a configuration with 13 stages is almost equivalent to increase the number of stages from 13 to 18. Throughout the case study, the absorber efficiency, lean/rich amine heat exchanger minimum temperature approach, all flue gas parameters and lean amine content were all kept constant. The lean amine feed in ADJ-1, the desorber input temperature in ADJ-2, the flow rate of inlet cooling water in the inlet heat exchanger in ADJ-3 and the mass balance of makeup MEA and water in the makeup streams spreadsheet had to be adjusted to maintain the specification values.

2.4. Parameter variation of absorber inlet temperature

An analysis was conducted to adjust the flue gas inlet temperature to the absorber column. A high column temperature will increase the absorption rate and reduce the CO_2 solubility, so it is expected that the inlet temperature has an optimum. This is done in ADJ-3 by altering the cooling water input flow rate and as a result also changing the absorber inlet temperature. The lean amine composition was kept constant (by defining the MakeUp Streams spreadsheet), but the lean amine flow rate was adjusted in ADJ-1 for each case to obtain the desired CO_2 removal efficiency. The ADJ-2 operates to keep the ΔT_{min} constant in the lean /rich amine heat exchanger.

It is possible to specify the Murphree efficiency for each absorber stage. The Murphree efficiency must be adjusted for each new inlet temperature, which makes this calculation complex. The Murphree stage efficiency was adjusted to account for the impacts of varying temperature profiles in the absorber column at various input gas temperatures. Øi (2012) has made a computational approach for estimating the Murphree stage efficiency as a function of temperature for absorber top and bottom conditions. Based on this calculation scheme, the Murphree efficiencies were computed only for the top-, bottom-, and maximum temperature stages, and the intermediate stage temperatures have been obtained

using a linearization between these temperatures as done in Kallevik (2010).
After calculating the average Murphree efficiency for each inlet flue gas temperature, an equation for the relationship between the inlet temperature and Murphree efficiency was made. Another spreadsheet was created to export the calculated stages efficiency to the absorber after changing the incoming flue gas temperature from 30 to 50 °C in the case study.

3. Cost estimation procedures and assumptions

3.1. Equipment dimensioning and assumptions

The mass and energy balances from the Aspen HYSYS process simulations were used to dimension all the equipment as done in previous studies (Øi *et al.*, 2022).

The diameters of the absorption and desorption columns were evaluated from the gas stream's volumetric flows. These were based on superficial gas velocities of 2.5 m/s and 1 m/s respectively as done in earlier studies (Aromada & Øi, 2017). In the base case, 15 packing stages were specified for absorber, and 10 for the desorber. Each packing stage in the absorber and desorber were assumed to be 1 m high (Aromada *et al.*, 2020). Structured packing was specified for better operational cost due to pressure drop (Choi *et al.*, 2005). To estimate the tangent-to-tangent height of the absorber, the packing, liquid distributors, water wash, demister, gas inflow and outflow and sump were all considered. The condenser inlet, packing, liquid distributor, gas input and sump were taken into account in estimation of the desorber tangent-to-tangent height (Ali, 2019; Øi *et al.*, 2021). The packing height was given from a design of a wash tower in the catalog (Sulzer Chemtech, 2021). Thus, 35 m and 25 m were arrived at for the tangent-to-tangent heights of absorber and desorber respectively.

The separator was sized using Souders Brown's equation with a k-factor of 0.15 m/s and a height to diameter ratio of 1. The heat duties obtained from the process simulations were used to size the heat exchange equipment. The overall heat transfer coefficients specified are 1.20 kW/(m²·K) for the reboiler, 0.73 kW/(m²·K) for the lean/rich heat exchanger, 0.80 kW/(m²·K) for the amine cooler, and 1.00 kW/(m²·K) for the condenser as in Aromada *et al.* (2022b). The pumps, compressor and fan were sized based on their duties with efficiency 75 %.

3.2. Capital cost estimation method

The Enhanced Detailed Factor (EDF) method (Ali *et al.*, 2019; Aromada *et al.*, 2021) was applied for the estimation of the CO_2 capture plant's capital cost. As a detailed factor approach, the installed cost of each equipment is estimated based on variable installation factors that depends on each equipment cost. The capital cost of the CO_2 capture plant is then the sum of all equipment installed costs. The updated EDF factor list is published in (Aromada *et al.*, 2021).

Each equipment unit delivered cost was obtained from Aspen In-plant Cost Estimator (v.12). This is based on the capacity or size of each of the equipment units as determined from the dimensioning process. The cost currency and cost year were Euro (€) and 2019. The default location in Aspen In-Plant Cost Estimator, Rotterdam, was assumed in this work. The equipment units were assumed to be constructed from stainless steel (SS316). To apply the EDF method, the cost of the equipment units must be converted from their costs in the original material of construction. The cost (EC_{SS}) of an equipment unit in stainless steel (SS) needs to be converted to its cost (EC_{CS}) in carbon steel (CS). This is implemented by applying a material factor (f_{mat}) where CS is the reference material. The cost of each equipment unit constructed in welded SS is divided by a material factor of 1.75 to convert it to the corresponding cost in CS material. While the material factor for units manufactured in machined SS, e.g. pumps, is 1.30. Then, the total installation factor $(F_{T,CS})$ and piping subfactor (f_{pp}) in CS for each equipment unit are obtained from the EDF factor lists (Aromada *et al.*, 2021). They are then converted to total installation factor in SS $(F_{T,SS})$ as shown in equation (1):

$$F_{T,SS} = \left[F_{T,CS} + \left\{(f_{mat} - 1)\left(f_{eq} + f_{pp}\right)\right\}\right] \qquad (1)$$

Where f_{eq}= equipment factor = 1.0

The total equipment installed cost (*EIC*) is estimated as follows:

$$EIC_{SS} = F_{T,SS} * EC_{CS} * (No.of\ units) \qquad (2)$$

Then the total installed cost (CAPEX) with cost year of 2019 is:

$$CAPEX = \sum(EIC_{SS}\ for\ all\ equipment) \qquad (3)$$

The capital cost of the CO_2 capture plant is then escalated from 2019 to 2021 using a consumer cost index from Statistisk Sentralbyrå (SSB). A Norwegian cost index is selected because the detailed factors were originally based on Norwegian currency.

During optimization or sensitivity analysis, where a parameter is varied, the capacities/sizes of some equipment will change. Therefore, there is a need to estimate new delivered cost for the equipment units due to the resulting changes in size/capacity. This is automatically estimated based on the Power law using an exponent of typically 0.65, from the previous cost obtained from Aspen In-Plant Cost

Estimator database as done in (Aromada *et al.*, 2022a, Aromada *et al.*, 2022b; Øi *et al.*, 2022).

3.3. Operating cost estimation and assumptions

The annual operating cost in this work is the sum of the fixed operating cost and variable operating costs. The variable operating cost was estimated from equation (4):

$$Annual\ variable\ cost \left(\frac{€}{yr}\right) = Consumption \left(\frac{unit}{hr}\right) \times \frac{Operating\ hours}{year} \times unit\ cost \left(\frac{€}{unit}\right) \quad (4)$$

The assumptions used for estimating the annual operating cost are presented in Table 2. The values are similar to values used in earlier work like Aromada et al. (2021). The steam cost is set to 25 % of the electricity cost because steam can be converted to electricity with an efficiency of order of magnitude 25 %.

Table 2: Annual operating cost assumptions.

Item	Unit	Value
Operating lifetime	[Year]	25[1]
Annual hours of operation	[h/year]	8000
Electricity cost	[€/kWh]	0.06
Steam cost	[€/kWh]	0.015
Cooling water cost	[€/m^3]	0.022
Water process cost	[€/m^3]	0.203
MEA cost	[€/ton]	1450
Maintenance cost	[€/year]	4% of CAPEX
Operator cost (6 oper)	[€/year]	80414(*6)
Engineer cost (1 eng)	[€/year]	156650

[1] 2 years construction + 23 years operation

3.4. CO_2 capture annualized cost

The economic key performance indicator in this work is CO_2 captured cost. This was estimated as:

$$CO_2\ captured\ cost = \frac{Total\ annual\ cost}{Mss\ of\ Captured\ CO_2/year} \quad (5)$$

$$Total\ annual\ cost = Annualized\ CAPEX + Yearly\ OPEX \quad (6)$$

$$Annualized\ CAPEX = \frac{CAPEX}{Annualized\ factor}$$

$$Annualized\ factor = \sum_{i=1}^{n} \left[\frac{1}{(1+r)^n}\right] \quad (7)$$

Where n is the plant lifetime, 25 years which includes 2 years for the plant's construction. And r is the discount rate and was assumed to be 7.5 %.

4. Results and Discussion

*4.1. **Base case cost results***

The overall equipment cost was calculated to 110 MEUR, and the absorber is the costliest equipment, accounting for 54% of the total cost. This is traditional in other calculations (Ali 2019; Aromada *et al.*, 2021). The structured packing cost accounts for 55 percent of the absorber's total cost.

The total operational expenditure (OPEX) for the Base case was calculated to 29 MEUR/yr. Steam is the costliest utility for this facility, costing 15 MEUR each year. The steam usage is calculated to 3.75 GJ/ton CO_2 captured and this is in line with values in literature (Choi et al., 2005; Øi, 2012).

4.2. Optimization of minimum ΔT approach

CO_2 captured cost and energy consumption as a function of ΔT_{min} is shown in Fig. 3. It shows a flat minimum between 11 and 15, and a minimum at 13 K. Fig. 3 is based on an automated case study in Aspen HYSYS. The simulations were also calculated manually, obtaining a smoother curve because all the parameters could be adjusted more accurately by trial and error. The results were similar, but the optimum ΔT_{min} was calculated manually to 12 K. Similar values have been calculated in several works (Øi, 2012; Shirdel *et al.*, 2022). In the case of using plate heat exchangers, the optimum ΔT_{min} will be less than 10 K.

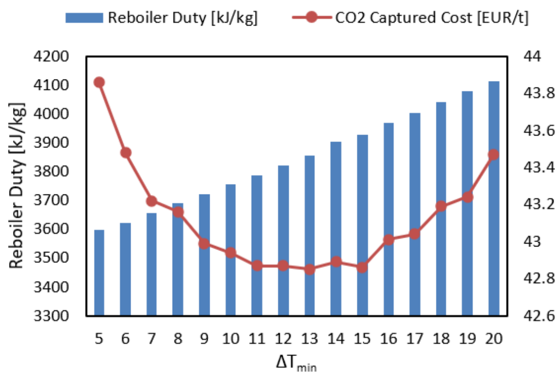

Figure 3: CO_2 captured cost and energy consumption as a function of ΔT_{min} (from Shirdel, 2022).

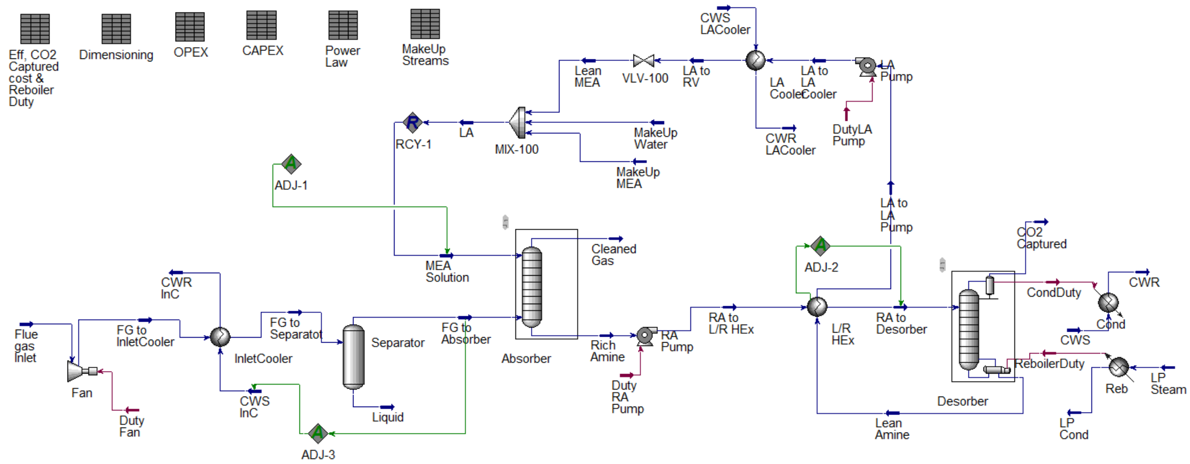

Figure 2: Aspen HYSYS flow sheet for the Base case simulation (from Shirdel, 2022).

4.3. Optimum absorber height

CO_2 captured cost and energy consumption as a function of absorber packing height is shown in Fig. 4. Results for both manual and automatic calculation are shown. Also here, the manual simulations give a smoother curve. However, the resulting optimum absorption height is 15 meters for both manual and automatic optimization. This is in the order of magnitude similar to earlier works where optimum packing height have been calculated to 20 meters (Mores *et al.*, 2012), 19 meters (Agbonghae *et al.*, 2014)) 15 meters (Aromada and Øi, 2017) and 19 meters (Shirdel *et al.*, 2022). All the heights were structured packing except for Mores et al. (2012) which was based on random packing.

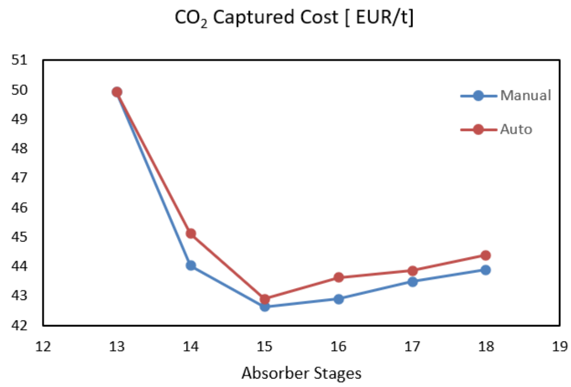

Figure 4: CO_2 capture cost as a function of absorber packing height (from Shirdel, 2022).

4.4. Optimum inlet gas temperature

To perform a reasonable optimization of the inlet gas temperature, the temperature dependence of the absorption efficiency must be included. In Fig. 6, the temperature and Murphree efficiency for the different absorption stages have been calculated. The Murphree efficiencies were calculated by the methods specified in Chapter 2, and one iteration was performed to include the effect of temperature on the calculated Murphree efficiencies from the first iteration.

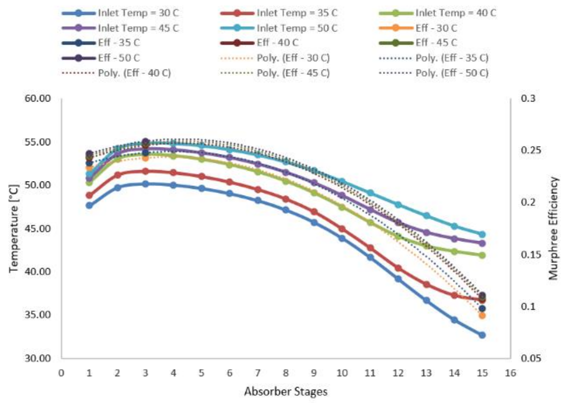

Figure 6: Murphree efficiency as a function of absorber stage and temperature (from Shirdel, 2022).

For each inlet gas temperature, an average Murphree efficiency was calculated by a fitted polynomial.

$$E_M = - 0.00004T^2 + 0.0041\ T + 0.08 \qquad (8)$$

A preliminary optimization was performed by manual simulations of the CO_2 capture cost with 5 K steps for 15 and 13 absorption stages. The lowest cost case was found at 13 stages (meter of packing). The optimum was then calculated automatically in a case study for 13 absorption stages with temperature steps of 1 K in Fig. 7.

Fig. 7 shows that it is possible to calculate the optimum inlet gas temperature automatically. The curve is not very smooth, and this indicates that there are some inaccuracies in the calculations. To improve this, a possibility is to adjust the tolerances in the Aspen HYSYS simulation tool. This was evaluated by Øi et al. (2021). The most optimum point at the curve is for an inlet gas temperature of 34 °C. There are not found many numbers to compare with in literature, but Øi (2012) calculated an optimum between 33 and 35 °C.

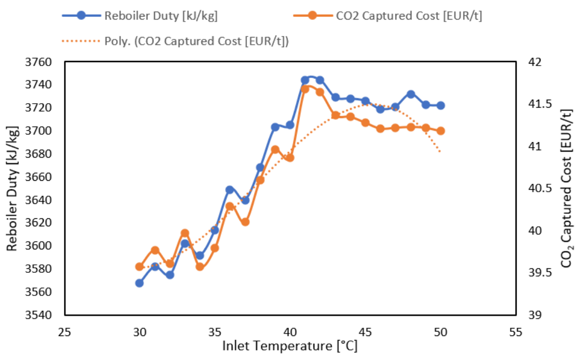

Figure 7: Optimization of inlet gas temperature (from Shirdel, 2022).

4.5. Optimization of other and several parameters

In this work, emphasis has been on the optimization of packing height, minimum temperature approach and inlet gas temperature. Other works have emphasized optimization of other parameters as absorber gas velocity and pressure drop (Park and Øi, 2017), CO_2 capture rate (Mores *et al.*, 2012) and lean loading (Agbonghae *et al.*, 2014). Optimization of these parameters are most often not independent. A high % CO_2 capture rate will e.g. give a lower optimum CO_2 loading.

Simultaneous optimization of several parameters have been evaluated by Mores *et al.* (2012) and Agbonghae *et al.* (2014). Mores *et al.* (2012) used a methodology based on Murphree efficiencies, and Agbonghae *et al.* (2014) based the work on rate-based modelling in Aspen Plus including the Aspen Plus Economic Analyser.

Such simultaneous optimization raises challenges for future work in complexity, accuracy, consistency and robustness of the calculations.

6. Conclusion

The case study function in Aspen HYSYS can be used to perform several simulations by changing one parameter at a time. The ΔT_{MIN} was optimum at 13 K (a flat optimum between 11-15 K) giving 42.8 EURO/ton CO_2. The case study function cannot be used to vary the number of stages in a column. However, the packing height was varied in an automated case study by increasing the Murphree efficiency of one stage gradually from 0.15 to 0.9. The optimum packing height at 15 meter (15 stages with 0.15 stage efficiency) gave 42.6 EURO/ton. Inlet temperature was optimized using the case study model where the Murphree efficiency was calculated as a function of temperature. Optimum inlet temperature was obtained at 34 °C, and the cost was reduced to 39.6 EURO/ton CO_2. The optimums agree well with earlier calculated optimum parameter values.

This study demonstrates that it is possible to calculate the optimum packing height and inlet temperature automatically by varying the Murphree efficiency in a case study function.

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