Process Simulation and Automated Cost Optimization of CO_2 Capture Using Aspen HYSYS

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Abstract

A standard process for CO_2 capture based on absorption in mono ethanolamine (MEA) has been simulated and cost estimated with an equilibrium-based model in Aspen HYSYS™. The aim has been to calculate cost optimum process parameters and evaluate the possibility of automated cost optimization using a spreadsheet facility. An Excel spreadsheet is used for dimensioning and cost estimation of the specified process. New in this work is that Visual Basic for Application (VBA) was used to automatically update installation factors for next iteration based on cost calculations in previous iteration. The equipment cost was obtained from the Aspen In-plant Cost Estimator™, and an enhanced detailed factor (EDF) method was used to estimate the total investment cost. The optimum process was found as the process with minimum calculated total cost. The cost optimum process parameters for the standard process were calculated to 15 m absorber packing height, 9 °C minimum approach temperature and 2.2 m/s superficial gas velocity through the absorber. With this approach, iterative cost estimation and optimization of CO_2 absorption and desorption processes can be performed automatically.

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

1. Introduction

1.1. Aim

One aim of this work was to calculate cost optimum process parameters for a traditional amine based CO_2 capture process. Another aim was to evaluate the possibility of automated cost optimization using a spreadsheet facility. An Excel spreadsheet is traditionally used for dimensioning and cost estimation of the specified process with optimization performed by minimizing the total cost calculated in the spreadsheet. New in this work is that Visual Basic for Application (VBA) was used to automatically update installation factors for next iteration based on cost calculations in previous iteration.

1.2. Literature

There is a large number of papers on cost estimation of CO_2 capture plants (Rao and Rubin, 2002; Rubin *et al*., 2013; van der Spek *et al*., 2019). Some of these are based on a combination of process simulation and cost estimation (Abu-Zahra *et al*., 2007; Amrollahi *et al*., 2012; Nwaoha *et al*., 2018).

This work is a further development of earlier works at the Telemark University College and the University of South-Eastern Norway (USN). The projects have been focused on process simulation, equipment dimensioning, capital and operating cost estimation, and cost optimization of CO_2 capture processes using the process simulation tool Aspen HYSYS. Some of the previous works are Kallevik (2010), Øi (2012), Park and Øi (2017), Aromada and Øi (2017), and Øi *et al.* (2021).

The cost estimation part has been based on the Enhanced Detailed Factor (EDF) method (Ali *et al*., 2019; Aromada *et al*., 2021). While this method has several advantages, the time required to implement the detailed installation factors in capital cost estimation is a drawback. This becomes cumbersome when there is a need to run several process simulations by varying a process parameter followed by cost estimation for each iteration.

Recently, the focus has been on automatic process simulation combined with cost estimation for fast cost optimization of CO_2 capture processes in Aspen HYSYS (Haukås, 2020; Øi *et al*., 2021). The Iterative Detailed Factor (IDF) scheme was then developed (Aromada *et al*., 2022a). The IDF scheme was applied for several minimum temperature approach cost optimization studies in (Aromada *et al*., 2022a). However, there was yet a need for manual observation for implementing any change required in the detailed installation factors and subfactors whenever process parameters are varied for subsequent simulation of the CO_2 capture process. Therefore, there is a need to make the entire process simulations, equipment dimensioning and cost estimation automatic, without requiring any manual input as done in the IDF scheme mode of implementation (Aromada *et al*., 2022a). This was accomplished in this work by linking Aspen HYSYS simulation spreadsheets with Microsoft Excel by a VBA code. This has been discussed by Sharma and Rangaiah (2016).

The Aspen HYSYS library was activated in Microsoft Excel from the developer tab > visual basic > tools> and preference (Rangaiah, 2016; Rahmani, 2021). The Aspen HYSYS root needs to be inserted into a Microsoft Excel sheet and it should be updated for each model. The Aspen HYSYS application should be closed during the process. The VBA script was developed for coupling the Aspen HYSYS and Microsoft Excel spreadsheets. The code imports equipment prices from the Aspen HYSYS spreadsheet into an Excel spreadsheet for cost estimation and optimization. At the same time, the right equipment units' installation factors/sub-factors are automatically imported from the Microsoft Excel sheet into the Aspen HYSYS spreadsheet. By this, the EDF method is simply and automatically implemented very fast without errors in the selection of the detailed installation factors/subfactors. The code and more details are documented in (Rahmani, 2021).

With this new approach of involving a VBA code, human errors in selecting EDF method installation factors and subfactors for different equipment are eliminated. And most importantly, each time a new process simulation is performed, the costs are automatically available without requiring any form of manual inputs.

With this work, process simulation based CO_2 capture process parameter cost optimization studies and sensitivity analysis can be conducted quickly and obtain reasonably accurate results. This paper documents cost optimization studies conducted with this new approach and comparison with other works. This work is based on the Master thesis work of Rahmani (2021).

1.3. Process Description

Prior to the CO_2 capture process, the flue gas is cooled in a direct contact cooler (DCC) with circulating water before it is sent to the absorption column. The amine with absorbed CO_2 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 CO_2 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 before it again enters the absorption column.

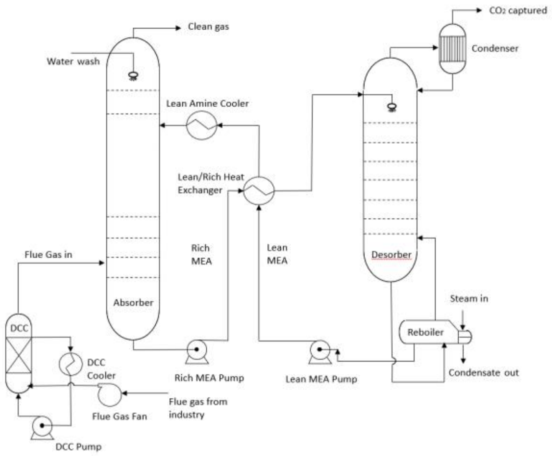

Figure 1: Process flow diagram of a standard amine-based CO_2 capture process (Aromada *et al*., 2020).

2. Specifications and simulations

2.1. Specifications and simulation of standard CO_2 capture process

Specifications for the base case are given in Tab. 1. In the base case, 85 % CO_2 removal efficiency and a minimum approach temperature of 10 °C was achieved in the lean/rich heat exchanger. Aspen HYSYS version 11 was used with the Acid Gas package as the recommended equilibrium model by Aspen HYSYS.

The calculation sequence is similar to earlier works (Øi and Haukås, 2021). The calculation strategy is based on a sequential modular approach (Kisala *et al*., 1987; Ishii and Otto, 2008). The calculation starts with the flue gas inlet stream and a guessed amount of the lean amine stream. After calculation of the DCC and the absorption column, the amine/amine heat exchanger is calculated based on a guessed (or specified) temperature in the stream from the desorber. The temperature can be adjusted in an adjust block to obtain a specified minimum temperature approach. After calculation of the desorber, the lean amine pump and the amine/amine heat exchanger the lean amine cooler is calculated to give an updated lean amine amount and composition.

The updated lean amine amount and composition is checked in a recycle block with the amine stream from the last iteration.

Adjust and Recycle operations in the flowsheet are used to get an automated simulation model. An Adjust block is adjusting the minimum approach temperature in the lean/rich heat exchanger by varying the temperature on the hot side outlet. A Recycle block is adjusting the removal efficiency by varying the lean amine mass flow. The Aspen HYSYS flowsheet is shown in Fig. 2.

Water was added to the process (water make-up). The make-up water can be calculated by a material balance.

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

Parameter	Value
Inlet flue gas temperature [ºC]	110/40.0
Inlet flue gas pressure [kPa]	101/120
Inlet flue gas flow rate [kmol/h]	10910
CO_2 content in inlet gas [mole %]	3.3
Water content in inlet gas [mole %]	6.9
Lean amine temperature [ºC]	40.0
Lean amine pressure [kPa]	101.0
Lean amine rate [kg/h]	132100
MEA content in lean amine [mass %]	22.5
CO_2 content in lean amine [mass %]	3.5
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 [ºC]	103.6
Number of stages in desorber [-]	6
Murphree efficiency in desorber [m^{-1}]	0.5
Reflux ratio in stripper [-]	0.3
Reboiler temperature [ºC]	120.0
Lean amine pump pressure [kPa]	500.0

2.2. Parameter variations

10 stages, 85 % removal efficiency and 10 °C as minimum approach temperature were specified in the base case simulation. For parametric studies, the packing height and minimum approach temperature were varied. The gas velocity through the absorber column and the pressure drop were also varied.
The Case study function in Aspen HYSYS was used to perform a series of calculations automatically. An important restriction is that when using the Case study function, it is not possible to perform other adjustments for each new parameter value.

2.3. Process convergence and stability

A Recycle block and an Adjust function were used in the Flowsheet calculation. The Modified Hysim Inside-Out algorithm with adaptive damping was used according to a recommendation by Øi (2012). This is the algorithm to solve the material, enthalpy and equilibrium equations in a column simulation. Stable convergence is especially important when running a Case study in Aspen HYSYS for the purpose of optimization.

3. Cost estimation procedures and assumptions

3.1. Equipment dimensioning and assumption

The equipment was dimensioned using the mass and energy balances obtained from the process simulations as done in previous works (Øi *et al.*, 2021).
The absorber was specified to have 10 stages and the desorber 6 stages (Aromada and Øi, 2017). Each stage of both columns was assumed to be 1 meter (Aromada *et al*., 2020). A constant stage (Murphree) efficiencies of 0.15 and 0.5 were specified for the absorber and the desorber respectively (Aromada *et al.*, 2022b). Structured packing was specified for both the absorber and desorber. Superficial gas velocity of 2.5 m/s was applied to estimate the diameter of the absorber (Øi *et al*., 2020). For the desorber, the desorber was evaluated using a superficial gas velocity of 1 m/s (Park and Øi, 2017). The tangent-to-tangent shell height of the absorber was specified to be 40 meter (Aromada *et al.*, 2022a). A tangent-to-tangent shell height of 15 m was used for the desorber. The height in both columns were necessary to account for distributors, water wash packing, demister, gas inlet, outlet and sump.
The sizing of the direct contact cooler and the flash tank were based on Souders Brown’s equation with k-parameter 0.15 and 0.075 respectively. The heat exchange equipment units were dimensioned based on the heat exchange areas calculated from the heat duties. The overall heat transfer coefficient of 500 W/(m^2K), 800 W/(m^2K), 800 W/(m^2K), and 1000 W/(m^2K) were specified for the lean/rich heat exchanger, lean amine cooler, reboiler and condenser respectively (Aromada *et al*., 2020).
The pumps were specified as centrifugal pumps with 75 % adiabatic efficiency. They were sized based on flow rate and duty.

3.2. Capital cost estimation methods

The capital costs were estimated using the Enhanced Detailed Factor (EDF) method (Ali *et al*., 2019; Aromada *et al*., 2021). The total capital cost is the sum of all the equipment installed costs. The EDF updated installation factors for 2020 by Nils Eldrup was used (Aromada *et al*., 2021).
A traditional factor method for cost estimation is based on a table of factors multiplying the purchased cost of each type of equipment unit. In a detailed factor method, the total factor for each type is the sum of contributions from e.g. installation, electrical, instrumentation, administration etc. In the EDF method, these detailed factors are also dependent on the size and cost of the purchased equipment, so that the factors may change from one iteration to the next in an optimization procedure.

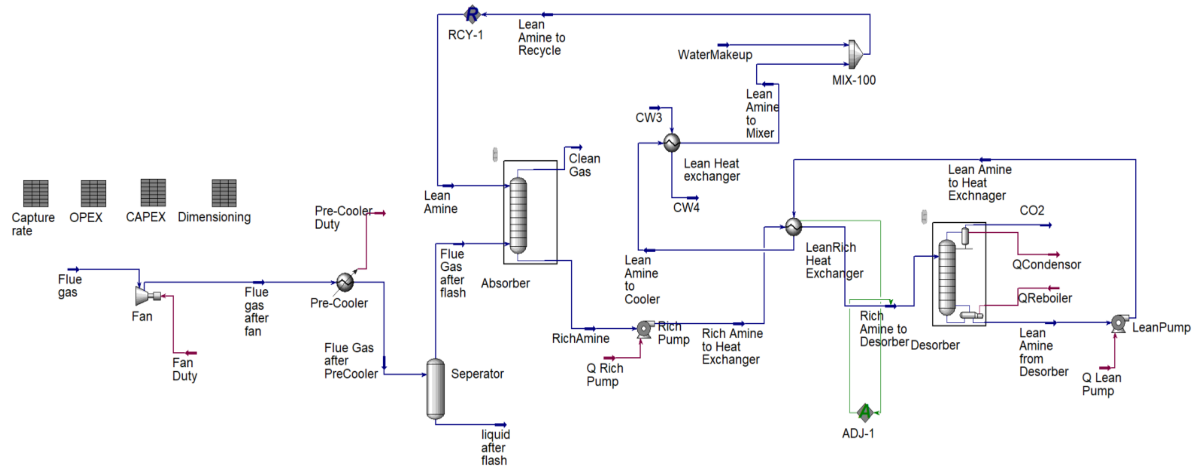

Figure 2: Aspen HYSYS flow-sheet of the base case simulation (Pouya, 2021).

The cost of each equipment was obtained from Aspen In-plant Cost Estimator (v.10), based on the sizes estimated. The cost currency is in Euro (€) and the cost year is 2016. The default location for Europe, Rotterdam was selected in this study. Stainless steel (SS316) was specified for all equipment. Welded equipment has a material factor of 1.75. The seamlessly manufactured equipment, the pumps and fan have a material factor of 1.3 (Øi *et al.*, 2021).
Since this work is aimed at automatic cost estimation, the capital cost is initially estimated based on equipment costs obtained from Aspen In-Plant Cost Estimator. Subsequent equipment cost is then estimated automatically based on the Power law. The Power law is based on the assumption that the cost ratio of two sizes of a unit is proportional to the dimension ratio raised to a power factor (typically 0.65). The installation factors and subfactors are also automatically implemented in each simulation iteration by the aid of the VBA code which connects Aspen HYSYS spreadsheets with Microsoft Excel spreadsheet.
The economic assumptions used for the capital cost estimation are summarized in Tab. 2 (Rahmani, 2021).

Table 2: Cost calculation specifications (Rahmani, 2021).

Parameter	**Value**
Plant lifetime	20 years
Discount rate	8.5 %
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
Currency exchange rate 2016	9.21
Cost index 2016	103.6
Cost index September 2020	111.3

3.3. Operating cost estimation and assumption

The annual operating cost in this work was limited to cost for consumption of steam, electricity, cooling water and an annual maintenance cost as done in (Aromada and Øi, 2017). The electricity consumption was based on the pump duties obtained from Aspen HYSYS. Similarly, the steam consumption was based on the reboiler steam duty in kW. The annual hours of operation were assumed to be 8000 hours/year. The annual maintenance cost was specified as 4 %.

3.4. Net present value

The cost metric in this work for cost optimization is negative net present value (NPV) as done in (Haukås, 2020). The NPV is the sum of investment cost and the operation cost for each year in the plant lifetime. 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. The optimum solution can then be found by the simulation giving the lowest NPV as shown in Fig. 3. For the case of optimizing the number of absorber stages, each calculation was performed independently by specifying the number of stages in each calculation.

4. Results and Discussion

4.1. *Base case cost results*

For the base case, the total cost (or negative NPV) was estimated to 401 mill. EURO. This is the sum of CAPEX and OPEX for a Plant lifetime of 20 years.

4.2. Optimization of minimum ΔT approach

The minimum temperature approach optimization for the process is shown in Fig. 3. The absorber packing height was 15 m in these optimizations. The optimum value at 9 K can be found as the one with minimum (negative) NPV. The cost optimum minimum temperature approach has been calculated in literature to values typically between 10 and 15 K. The differences are due to different ratios between cost of heat exchangers and cost of heat.

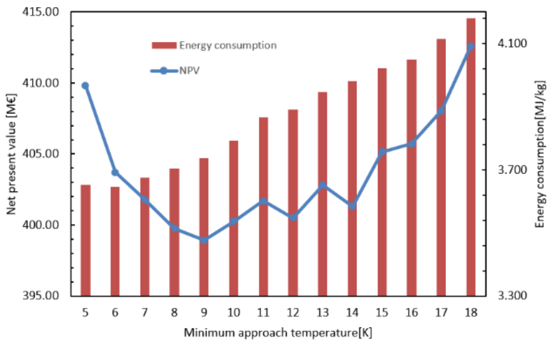

Figure 3: NPV and energy consumption as a function of ΔT_{min} with 85% capture rate, E_M = 0.25, 20 years calculation period, and 8.5% interest rate.

4.3. Optimum absorber height

The results from the optimization of the absorber packing height are given in Fig. 4. It shows an optimum for 15 stages equivalent to 15 meter packing height. This is similar to results in earlier work (Kallevik, 2010; Aromada and Øi, 2017; Øi *et al.*, 2020).

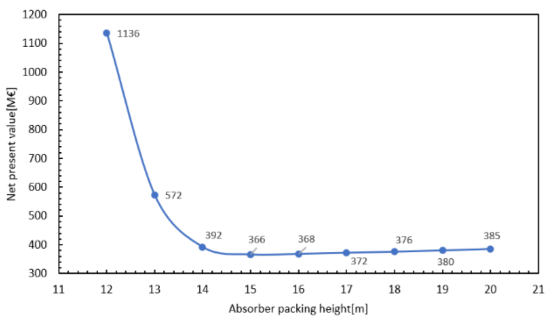

Figure 4: NPV as a function of absorber packing height with removal efficiency 85%, E_M=0.15, 20 years calculation period and 8.5% interest rate.

The minimum NPV when optimizing the absorber packing height is 366 mill. EURO. This is a cost reduction of 9 % compared to the base case.

4.4. Optimization of gas velocity

When the superficial velocity through the absorption column is increased, the cross section of the absorber decreases and reduces the cost, while the pressure drop increases and increases the cost. The result when varying the superficial velocity is given in Figure 5.

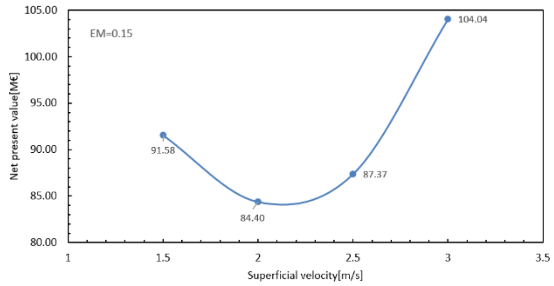

Figure 5: NPV as a function of superficial velocity with 85% capture rate, 20 years calculation period, and 8.5% interest rate and constant packing volume.

Fig. 5 shows an optimum for a gas velocity of about 2.2 m/s. This is a value close to values from Park and Øi (2017). There are not found other references in the open literature showing similar results to compare with.

5. Automation

5.1. Automation approaches

Automation of the simulations has been investigated, and results have been compared with manual simulations. Some of the input data should be changed in the simulations manually, which is time-consuming. Connecting Excel and Aspen HYSYS to transfer the data is the first step toward automating the process. In order to make the connection, one possibility is to use an Aspen simulation workbook and programming in Visual Basic. In addition, defining a case study in the Aspen HYSYS can be useful for automating the simulations.

The Aspen simulation workbook is an Excel feature that can be activated through Excel's settings. The Aspen HYSYS simulation model should be linked to Excel, under the simulation tab in the Aspen simulation workbook. Variables in the Aspen HYSYS simulation can be copied to the Aspen simulation workbook. In the scenario table, all of the input data are collected once, and the simulation runs one at a time.

ΔT_{min} is considered as input in the lean-rich heat exchanger. The capture rate and NPV are considered as outputs. In order to fix the capture efficiency at about 85%, a controller is added to the simulation.

Visual Basic for application (VBA) programming language in Excel is another method for automating the process and cost estimation in Aspen HYSYS. In Aspen HYSYS, it can be activated in Excel from the developer tab, visual basic, tools and preference. One of the most time-consuming steps in cost estimations is determining the correct installation factor e.g. from a table. With this approach VBA was used to automatically update installation factors for next iteration based on cost calculations in previous iteration.

5.2. Automatic optimization of ΔT_{min}

In Fig. 6, sensitivity analysis is performed comparing manual calculations and a case study including updated cost factors using the Visual Basic for Application approach as explained in subsection 5.1.

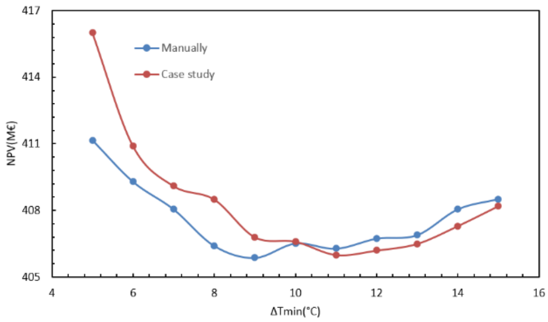

Figure 6: NPV as a function of ΔT_{min} with removal efficiency 85%, E_M=0.25, 20 years calculation period and 8.5% interest rate for case study(automatic) and manually, by using Aspen HYSYS model for ΔT_{min}=10°C.

The results are not exact equal for manual and automatic calculations. The accuracy is however reasonable, the difference in NPV is less than 1 %. The calculated optimum ΔT_{min} where 9 and 11 K, respectively. The study shows that it is possible to calculate reasonable optimums automatically.

5.3. Automatic optimization of column height and gas velocity

Automatic optimization of column height (number of absorber stages) is still a challenge. In Aspen HYSYS, the number of stages is specified in the simulation input and can only be changed manually. This is also the case for pressure drop in the absorber column which can be used for gas velocity optimizations. This limitation is not necessarily a restriction in the future versions or in other tools, so this is an interesting challenge for further work.

5.4. Automatic optimization of other processes

The automatic optimization method in this work is specific for a process simulation in Aspen HYSYS. In principle, this approach could be used for any process using any process simulation tool. However, the specific challenges using Aspen HYSYS is related to the limitations in Aspen HYSYS regarding possibilities for varying some specified parameters. Examples are the number of stages in a column and the pressure drop for a column stage which have to be specified manually.

6. Conclusion

The aim has been to calculate CO_2 capture cost optimum process parameters and evaluate the possibility of automated cost optimization using a spreadsheet facility. The adjust and recycle blocks are used to automate the energy and material balance for a specified simulation. An Excel spreadsheet is used for dimensioning and cost estimation of the specified process. New in this work is that Visual Basic for Application (VBA) was used to automatically update installation factors for next iteration based on cost calculations in previous iteration.

Equipment cost was obtained from Aspen In-plant Cost Estimator^{TM}, and an enhanced detailed factor method was used to estimate the total investment cost. Parametric studies of the absorber packing height and the minimum approach temperature in the main heat exchanger were performed at 85 % capture efficiency. The cost optimum process parameters for the standard process were calculated to 15 m absorber packing height, 9 °C minimum approach temperature and 2 to 2.2 m/s superficial gas velocity through the absorber.

With this approach, iterative cost estimation and optimization of CO_2 absorption and desorption processes can be performed automatically. Automatic optimization of some parameters like the number of column stages is a challenge because they must be specified manually.

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