Simulation Based Cost Optimization Tool for CO_2 Absorption Processes: Iterative Detailed Factor (IDF) Scheme

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Abstract

A simple, fast, and accurate process simulation based cost estimation and optimization scheme was developed in Aspen HYSYS based on a detailed factorial methodology for solvent-based CO_2 absorption and desorption processes. This was implemented with the aid of the spreadsheet function in the software. The aim is to drastically reduce the time to obtain cost estimates in subsequent iterations of simulation due to parametric changes, studying new solvents/blends and process modifications. All equipment costs in a reference case are obtained from Aspen In-Plant Cost Estimator V12. The equipment cost for subsequent iterations are evaluated based on cost exponents. Equipment that are not affected by any change in the process are assigned a cost exponent of 1.0 and the others 0.65, except the absorber packing height which is 1.1. The capital cost obtained for new calculations with the Iterative Detailed Factor (IDF) model are in good agreement with all the reference cases. The IDF tool was able to accurately estimate the cost optimum minimum approach temperature based on CO_2 capture cost, with an error of less than 0.2%.

Keywords: Carbon capture, Aspen HYSYS, simulation, cost estimation, techno-economic analysis

1 Introduction

Amine based post-combustion carbon capture technology is generally recognized as the most mature and promising technology that can be deployed industrially to reduce CO_2 emissions, which has become necessary for climate change mitigation (Karimi et al., 2011). The current challenge remains the economic implications of the huge energy consumption and the large capital investment requirements (Aromada and Øi, 2017).

This has led to several techno-economic studies. The focus of some of the research is on evaluating the representative costs for carbon capture and storage (CCS) (Stone et al., 2009). The objective of some other studies is on cost reduction and optimization (Fernandez et al., 2012).

Costs are projected to be reduced as research continues and as the first set of industrial CO_2 capture plants start operations (Sprenger, 2019; Aromada et al., 2021). The resulting new concepts and innovations will always be subjected to techno-economic evaluation and optimization or sensitivity analysis.

The common procedure for conducting carbon capture cost estimation and cost optimization studies is to import mass and energy balance data from a simulation software to Microsoft Excel or other applications for analysis each time a simulation is performed (Schach et al., 2010; Lassagne et al., 2013; Aromada and Øi, 2017).

Parametric variation or sensitivity analyses of costs that involve running the entire process simulation several times, and performing new equipment dimensioning, obtaining new costs for all the equipment, and recalculating the capital and operating costs can be very time consuming.

Applying a detailed factorial scheme for chemical plant's initial cost estimation has great advantages of accuracy and capabilities for different types of projects: new plant construction, retrofit or modification projects, small and large plant construction cost estimation (Gerrard, 2020; Ali et al., 2019; Aromada et al., 2021). However, it comes with much more work, and thus much more time to implement compared to methodologies that are founded on a uniform or single overall plant installation factor on all equipment irrespective of cost.

Therefore, there is a need to develop a cost estimation and optimization tool that will drastically reduce the overall economic analysis and optimization calculation time yet giving accurate cost estimates.

2 Model description

The iterative detailed factor (IDF) model is developed based on the Enhanced Detailed Factorial (EDF) method (Ali et al., 2019; Aromada et al., 2021). At Telemark University College and University of South-Eastern Norway (USN) there has been much focus on calculation of cost optimum parameters in CO_2 absorption-desorption processes. This involves varying different process parameters and different configurations (flowsheet modifications). The procedure commences from process development and simulation of the system's process flow diagram (PFD) to equipment dimensioning and cost estimation.

Each time any parameter is varied, this process is repeated. Consequently, in previous works (Kallevik, 2010; Aromada and Øi, 2017), there is a change in the cost of the equipment, when one of its parameters is being varied, but the costs of all other equipment are kept constant. Similarly, energy consumption by other equipment is also kept constant, while that of the equipment with parameters being optimized can vary. This procedure does not capture the effect of every change in the process caused by varying a specific parameter in the evaluation for optimum cost.

In addition, it is an aim to enable subsequent calculations of all the processes from simulations to cost estimation and optimization in not more than a minute.

The Enhanced Detailed Factorial (EDF) method used at USN has several advantages such as capability for new and modification projects (Aromada et al., 2021). Each equipment unit's installation factor is a function of its cost. This ensures that a very expensive equipment is not over-estimated, and a relatively cheaper equipment are not underestimated. This also comes with a challenge of relatively more work due to the details. Thus, it takes much more time to implement.

Therefore, the Iterative Detailed Factor (IDF) scheme was developed to consider all the effects caused by any parametric variation on the entire process, and to drastically reduce the time to implement cost estimation and other economic analyses of subsequent simulation iterations. The flowchart in Figure 1 explains how the scheme is developed and works. The arrows show how the process flows as well as where inputs come from and where they are used. The steps (and the directions of the arrows) are explained below:

1. Start: The PFD is developed and simulated in Aspen HYSYS.
2. Equipment dimensioning calculations based on mass and energy balances from the simulation are done in a separate Aspen HYSYS Spreadsheet as shown in Figure 2.
3. In the first simulation/cost estimation (base case), all equipment costs are obtained directly from a reliable (reference) source based on the calculated dimensions. In this work, equipment cost data were obtained from Aspen In-Plant Cost Estimator Version 12.
4. In subsequent iterations, when parameters are varied, a change to another solvent/blend is implemented, change in technical and/or economic underlying assumptions are made, or when the process configuration is modified, equipment cost is obtained by cost adjustment, utilizing cost exponents, capturing all the changes caused by the change of a process parameter or system as shown in equation (1):

$$EC_{new} = EC_{Base\ case}\left(\frac{Size_{new}}{Size_{Base\ case}}\right)^{n} \tag{1}$$

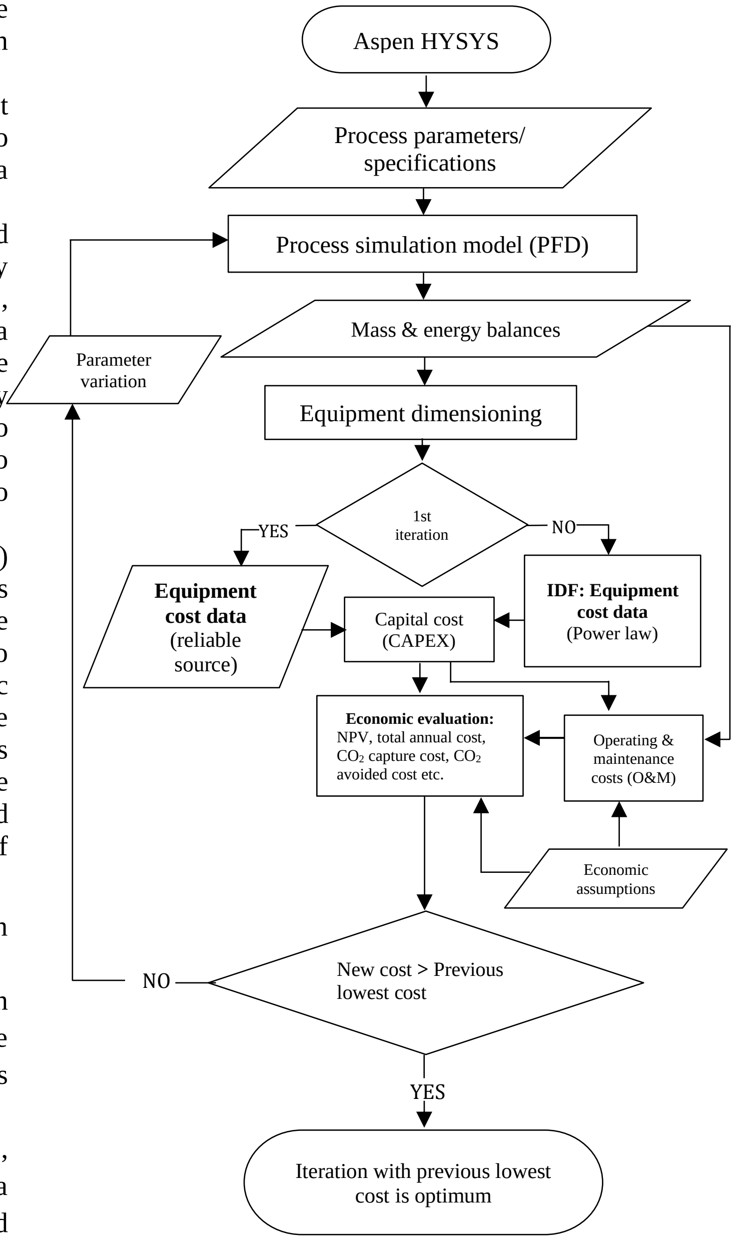

Figure 1. Flow chart describing the iterative detailed factor carbon capture cost optimization model

where $EC_{Base\ case}$ and $Size_{Base\ case}$ are equipment cost and size in the Base case obtained directly from the Aspen In-Plant Cost Estimator. EC_{new} and $Size_{new}$ are the new equipment cost and size for the new simulation evaluated using equation (1). And n is the cost exponent. All equipment costs in a reference case are obtained from a reliable source. The equipment cost for subsequent iterations are evaluated based on cost exponents (Power Law). Equipment that are not affected by any change in the process are assigned a cost exponent of 1 and the others 0.65, except for the absorber packing height (see Section 3.3).

5. All other costs and cost indices already programmed during the first iteration are automatically available after a minor check of the detailed installation factors. Further improvements can be achieved by avoiding manual adjustments of the installation factors between each iteration.
6. The cost optimum parameter is identified when the new cost estimated is less than the costs obtained in previous iterations, and in some cases, also less than cost obtained from subsequent simulations.
7. The capital cost, operating costs and other economic analysis are all done in separate Aspen HYSYS Spreadsheets as can be seen at the bottom of Figure 2.

2.1 Process simulation

The simulation sequence is the same as in (Aromada and Øi, 2015; Aromada et al., 2020a). The base case simulation was performed using the process specifications in Table 1. They are from a 400 MW natural gas combined cycle (NGCC) power plant. It is a 90% amine based CO_2 absorption and desorption in Aspen HYSYS Version 12.

Table 1. Specifications for simulation

Specifications	
Flue gas	
Temperature [°C]	80
Pressure [kPa]	121
CO_2 mole-fraction	0.0375
H_2O mole-fraction	0.0671
N_2 mole-fraction	0.8954
O_2 mole-fraction	0
Molar flow rate [kmol/h]	85000
Flue gas from from DCC to absorber	
Temperature [°C]	40
Pressure [kPa]	121
Lean MEA	
Temperature	40
Pressure [kPa]	121
Molar flow rate [kmol/h]	101595
Mass fraction of MEA [%]	29
Mass fraction of CO_2 [%]	5.30
Absorber	
No. of absorber stages	15
Absorber Murphree efficiency [%]	11- 21
ΔT_{min}, lean/rich heat exchanger [°C]	10
Desorber	
Number of stages	10
Desorber Murphree efficiency [%]	50
Pressure [kPa]	200
Reboiler temperature [°C]	120
Reflux ratio in the desorber	0.3
Temperature into desorber [°C]	104.6

The Aspen HYSYS process flow diagram (PFD) is shown in Figure 2. The absorption and desorption columns were simulated as equilibrium stages with 11 – 21% Murphree efficiencies (changing linearly from bottom to top) and 50% constant Murphree efficiency respectively.

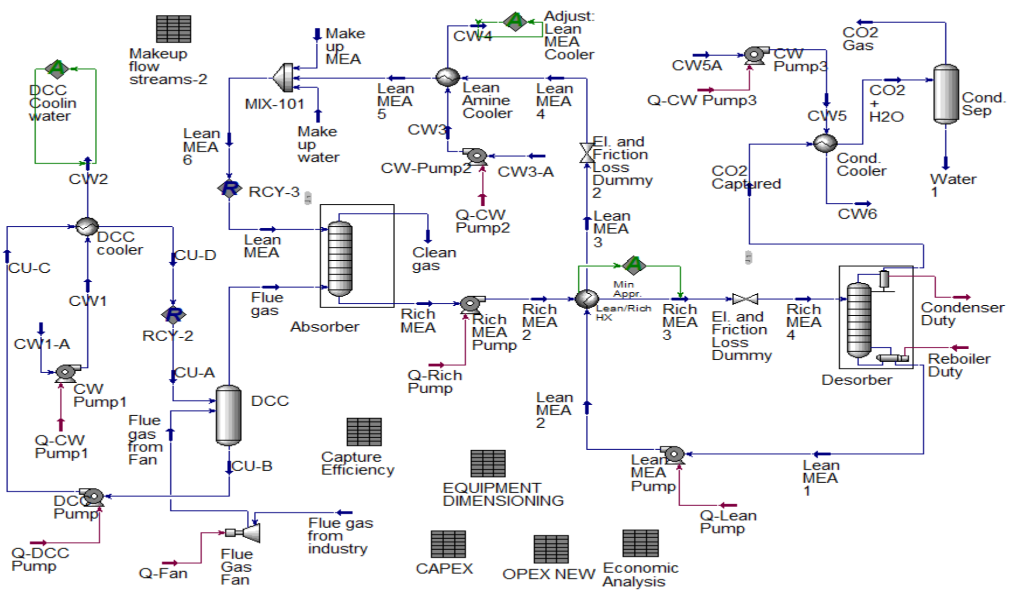

Figure 2. Aspen HYSYS process flow diagram (PFD) of the standard CO_2 capture process

2.2 Equipment dimensioning

Mass and energy balances from the simulations were used to size the equipment in Figure 2.

Table 2. Equipment dimensioning factors and assumptions

Equipment	Sizing factors	Basis/Assumptions
DCC Unit	Tangent-to-tangent height (TT), iterations: mass (*kg*); Packing height, internal and external diameters (all in [*m*]), iterations: volume (m^3);	Velocity using Souders-Brown equation with a k-factor of 0.15 m/s. TT =15 *m*, 1 *m* (structured) packing height/stage (4 stages)
Absorber		Superficial velocity of 2.5 m/s, TT=40 *m*, 1 *m* packing (structured) height/stage (15 stages)
Desorber		Superficial velocity of 1 *m/s*, TT=22 *m*, 1 *m* packing (structured) height/stage (10 stages)
Separator		Vertical vessel, Velocity using Souders-Brown
Lean/rich heat exchanger	Heat transfer area, A [m^2]	Duty, Q [*kW*], U = 0.73 $kW/m^2.K$ (Nwaoha et al., 2019). FTS-STHX
Reboiler		Duty, Q [*kW*], U = 0.8 $kW/m^2.K$, U-tube Kettle type
Condenser		Duty, Q [*kW*], U = 1.0 $kW/m^2.K$, UT-STHX
Coolers		Duty, Q [*kW*], U = 0.8 $kW/m^2.K$, UT-STHX
Pumps	Flow rate [*l/s*] and duty [*kW*], iterations: duty [*kW*]	Centrifugal. Efficiency = 0.75
Fans	Flow rate [m^3/h] and duty [*kW*], iterations: duty [*kW*].	Centrifugal. Efficiency = 0.75

The sizing factors, basis and assumptions for equipment dimensioning are summarized in Table 2. They are the same as in previous works (Aromada et al., 2020a) but on a different system. FTS-STHX refers to fixed tube-sheets Shell and tube heat exchanger, and the U-tube type is UT-STHX. More details on the equipment dimensioning can also be found in (Aromada et al., 2020; Aromada et al., 2021).

2.3 Capital Cost Assumptions

The capital cost in this work is the sum of each equipment installed cost. The IDF scheme is based on the EDF method (Ali et al., 2019; Aromada et al., 2021). All equipment is assumed to be manufactured from stainless steel (SS) with exception of the fan which is constructed from carbon steel (CS). Equipment costs in SS are converted to their corresponding costs in CS. Each equipment installed cost is obtained as a product of the equipment cost in CS and its individual detailed installation factor.

The cost year is 2020 and the cost currency is Euro (€). Therefore, the 2020 updated detailed installation list was used (Eldrup, 2020). The factors are derived based on 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.

2.4 Operating costs scope and assumptions

Operating costs in this work include cost for electricity, steam, cooling water, solvent, maintenance and salaries. The economic assumptions are tabulated in Table 3.

Table 3. Economic assumption for operating cost

	Unit	Value/unit
Operational hours	Hours/year	8 000
Steam	€/kWh	0.026
Electricity	€/kWh	0.059
Cooling water	€/m^3	0.075
Process water	€/m^3	6.77
MEA	€/m^3	1514
Maintenance	€	4% of TPC
Supervisor (1)	€	156 650
Operators (6)	€	80 000

3 Results and Discussion

3.1 Process Simulation Results

The specific reboiler heat obtained in the base case is 4.10 GJ/t CO_2, and the rich loading is 0.46. The rich loading is the mole ratio of CO_2 to the MEA in the rich stream exiting the absorber. The results have good agreement with literature. Sipöcz and Tobiesen (2012) calculated a reboiler heat of 3.97 GJ/t CO_2 and 0.47 rich-loading. In addition, Sipöcz et al. (2011) for an NGCC's exhaust gas also obtained 3.93 GJ/t CO_2 and 0.47 rich loading.

For a case with a minimum approach temperature of 5°C in the main heat exchanger, a reboiler heat of 3.78 GJ/t CO_2 and 0.47 rich loading were calculated. This is also close to the results obtained by Dutta et al. (2017), which are 3.70 GJ/t CO_2 reboiler heat and 0.47 rich loading.

3.2 Base Case Capital and Operating Costs

The capital cost estimated in the base case is €135 million. The capital cost in this work is limited to the total plant cost (TPC). It also does not include CO_2 compression or other flue gas pre-treatment sections other than the direct contact cooling loop. This is sufficient as all the sensitivity analysis conducted in this work are merely within the main CO_2 capture process between the absorber and the desorber. Nth-of-a-kind (NOAK) was also assumed. It is important to state that a first-of-a-kind (FOAK) plant would cost 115 – 155% of a NOAK plant (Boldon and Sabharwall, 2014; Aromada et al., 2020b). In a similar work (NOAK) that included the compression section, the TPC was estimated to €189 million (Aromada et al., 2021).

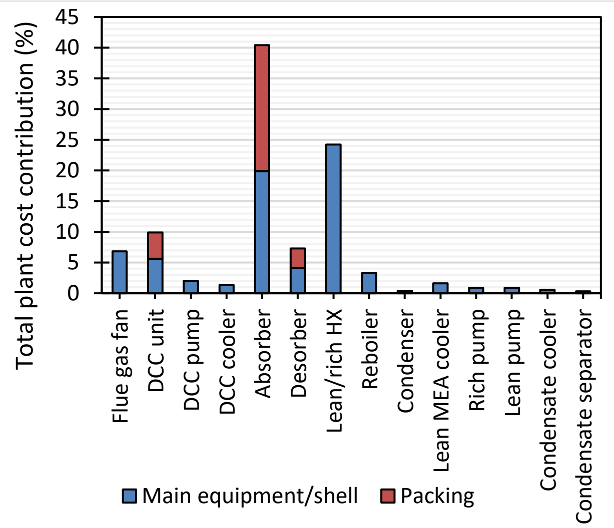

Figure 3. Capital cost distribution

The capital cost distribution is shown in Figure 3. It can be observed that the absorber and the lean/rich heat exchanger are the main cost contributors to the capital costs. Their contributions are 40% and 24% respectively. Therefore, the absorber and the main heat exchanger are the most important equipment for cost optimization in this capture process. Consequently, the IDF tool for process cost optimization based on process parameter variation was tested on the two equipment units for validation.

The cost of the lean/rich heat exchanger in initial cost estimation is a function of the required heat transfer area (m^2). The area varies much with the temperature difference (ΔT_{min}). The required area is doubled if the ΔT_{min} is 5°C instead of 10°C (Karimi et al., 2011). Therefore, ΔT_{min} has often been a very important process parameter to optimize in different solvent-based carbon capture processes (Aromada et al., 2020b; Aromada and Øi; 2017; Øi, 2012; Karimi et al., 2011).

In previous works, the absorption column, especially the packing height has been given attention for optimization, to reduce the entire cost of the process (Øi et al., 2020; Aromada and Øi, 2017; Kallevik, 2010).

3.3 Validation of the IDF Scheme: Capital Cost

To validate the accuracy of the scheme, it is important to perform cost estimation of the same process, with equipment cost data obtained from a reliable or reference source, and equipment costs estimated using the IDF scheme on the same process.

To evaluate the performance of the IDF scheme, equipment costs were first obtained from Aspen In-Plant Cost Estimator for each simulation iteration. These costs were used to estimate capital cost for each iteration, capturing the effect of the variation of a specific process parameter on all equipment in the process. These reference costs are referred to as the "original cost" since the equipment costs are directly obtained from a reliable cost database. This process is time consuming.

The IDF scheme is then applied for estimating the capital cost, operating cost, and CO_2 capture cost in each parameter variation simulation iteration. The IDF tool equipment costs were estimated from the base case equipment purchase cost based the Power law as described in Section 2.

The equipment costs in the IDF Scheme were calculated with a cost exponent of 0.65 for all the equipment that changes in size when a specific process parameter is varied, except for the absorber packing height. The larger the packing volume, the more the column and packing supports and auxiliaries are needed. Thus, costing the entire column may not necessarily follow economy of scale principle by using a cost exponent of 0.65. A range of cost exponents where then tested: 0.65, 0.85, 0.9, 1.0 and 1.1. To differentiate the results of each cost exponent, each cost exponent was designated PH-cost exponent. PH signifies packing height, which is being varied, while the number refers to the cost exponent used for estimating the new costs of the new packing size (volume). For example, in the case of PH-0.65 results, it means that as the packing height (PH) of the absorption column was varied between 12 *m* and 25 *m*, the costs of the new packing heights (12 *m*, 18 *m*, 20 *m*, 22 *m*, and 25 *m*) were estimated using a cost exponent of 0.65. New packing costs were also similarly estimated using cost exponents of 0.85 (PH-0.85), 0.90 (PH-0.90), 1.0 (PH-1.00), and 1.10 (PH-1.10). The results are plotted together and are compared with the original cost, that is the cost obtained directly from Aspen In-Plant Cost Estimator version 12.

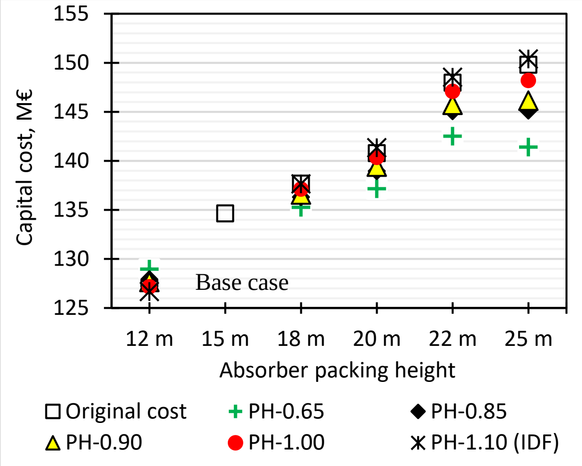

Figure 4. Impact of varying absorber packing height on the plant's capital cost with different cost exponents

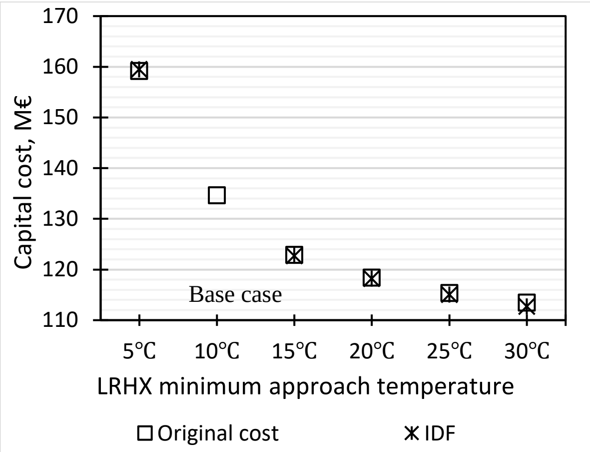

Figure 5. Comparison of IDF Scheme capital costs with reference capital cost when the temperature difference in the lean/rich exchanger is varied

Figure 4 shows that the cost exponent of 1.1 has the best agreement with the original cost for new sizes higher than the base case, and 0.85 for the size (12 *m* packing height) less than the base case (15 *m* packing height). However, cost exponent 1.00 also has a good agreement. Therefore, a cost exponent of 1.10 was used in the IDF scheme to estimate the cost of the absorber packing volume from the Base case (original cost) for higher volumes and 0.85 for volume less than in the base case where the absorber packing height is 12. The results suggest that due to the peculiarity of the cost of the packings/auxiliaries/supports/installations, not necessarily following economy of scale when the size of the column increases, new cost due to size adjustment using Power Law would require a cost exponent of 1.1 to minimize the estimation error or deviation from the original (reference) cost.

The ΔT_{min} of the main heat exchanger was varied from 5°C to 30°C in steps of 5°C. The IDF Scheme capital costs in each iteration were similarly estimated but with a cost exponent of 0.65 for all equipment apart from the columns and their packings, which were estimated with a cost exponent of 1 as they were kept constant. Varying ΔT_{min} will not have any effect on the absorber. Figure 5 presents the comparison of capital cost estimates from the IDF tool with the original capital costs. Original or reference costs are the cost obtained directly from Aspen In-Plant Cost Estimator. The agreement is quite good. The trend of the estimates is also similar to results in (Aromada et al., 2020b).

3.4 CO_2 Capture Cost

Trade-off analyses of the resulting capital and operating costs due to varying of the two process parameters were conducted, using the economic cost metric of CO_2 capture cost. This was estimated as follows:

$$CO_2\ capture\ cost\left(\frac{€}{tCO_2}\right) = \frac{Total\ annual\ cost(€)}{Mass\ of\ CO_2\ captured\ (tCO_2)} \quad (2)$$

where, the total annual cost is the sum of the annual capital cost and yearly operating expenses as done in (Aromada et al., 2020a). The results are presented in Figure 6 and Figure 7. The agreement with the original cost is very good. In Figure 6, IDF estimates used 0.85 as cost exponent for absorber packing height of 12 *m* and 1.1 for packing heights above that of the Base case (15 *m*) as explained in the previous section. However, capture cost was also estimated using 1.1 for 12 *m*, which is represented by a "red circle". The agreement is also good but using 0.85 is more accurate. This implies that the IDF scheme will still give good estimates if 1.1 is used as the cost exponent for all packing height iterations.

Figure 7 is specifically a cost optimization result. The cost optimum ΔT_{min} is 15°C which is the same cost optimum temperature difference calculated in (Aromada et al., 2020b) even though both process specifications, CO_2 concentrations and capture rates are different. Aromada et al. (2021) also calculated the cost optimum ΔT_{min} to be 15°C for a similar process but including CO_2 compression process. Kallevik (2010) estimated the minimum cost at 90 % CO_2 capture as in this study to be 15°C. The results obtained show that apart from drastically reducing the work and time required for cost estimation and cost optimization calculations in subsequent process simulation iterations, the IDF tool can give accurate or acceptable capital cost and operating cost.

The specific reboiler heat plot in Figure 7 indicates that the capital cost dominates at 5°C. The capital cost influence declines till the cost optimum, after which the energy cost (operating cost) begins to dominate.

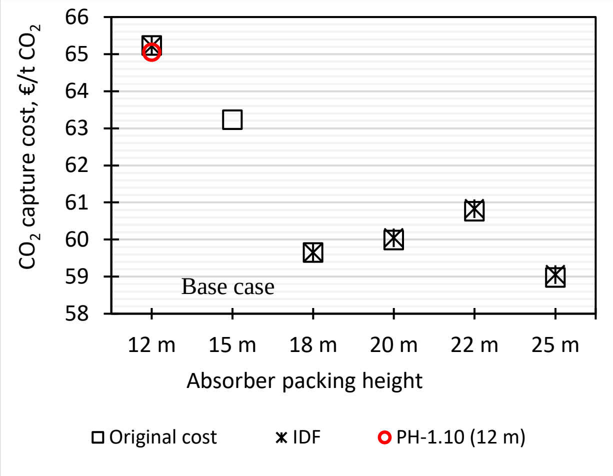

Figure 6. Impact of varying absorber packing height on CO_2 capture cost

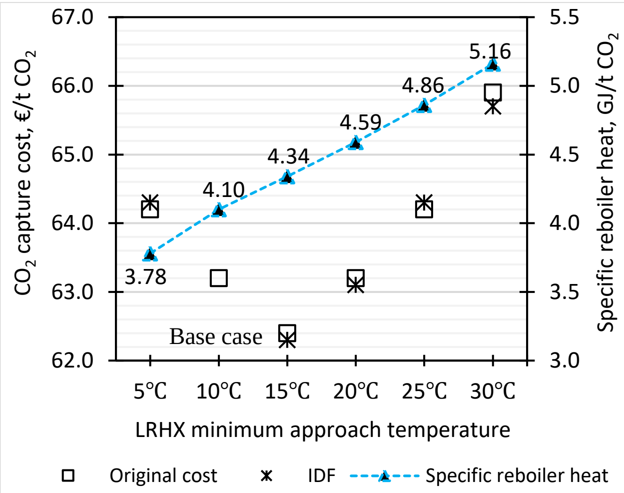

Figure 7. Impact of varying the minimum approach temperature in the lean/rich exchanger on CO_2 capture cost

3.5 Accuracy

We conducted an error analysis of the IDF tool using a simple percentage of differences between the IDF Scheme results and the original costs. This was performed as follows:

$$Error\ (\%) = \frac{(IDF\ result - Original\ cost)}{Original\ cost} \times 100 \quad (3)$$

A negative value indicates that the IDF Scheme estimate is less than the original or reference cost and vice versa. The IDF Scheme's errors in both the capital cost and CO_2 capture cost estimates for absorber packing height and lean/rich heat exchanger's temperature difference iterations are presented in Figures 8 and 9, respectively.

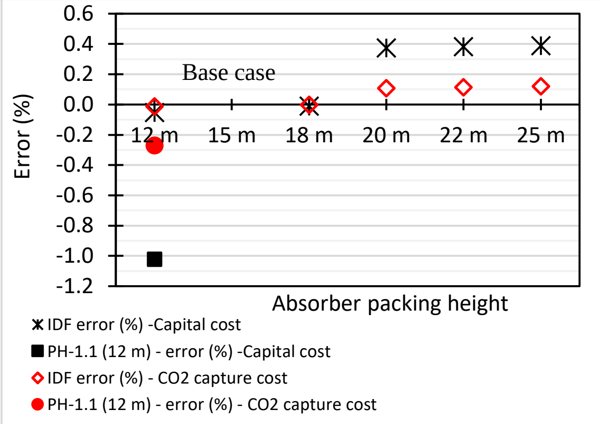

Figure 8. Error analysis of resulting capital costs by varying the absorber packing height

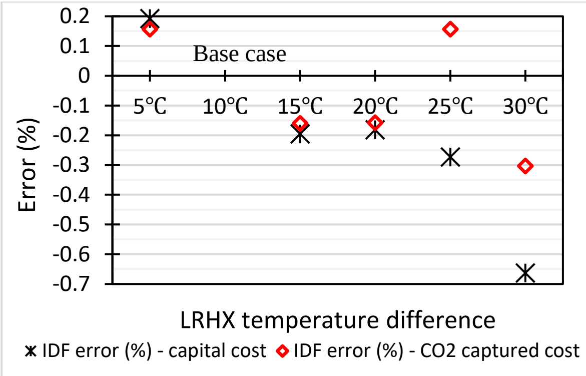

Figure 9. Error analysis of resulting capital costs by varying the minimum approach temperature in the lean/rich exchanger

In the case of varying the absorber packing height, the error in the capital cost estimates of the scheme is between 0.01 to 0.39%, while it is 0 to 0.12% for CO_2 capture cost (Figure 8). If 1.1 is used as cost exponent for 12 *m* which is less than the Base case size (15 *m*), the errors at that point increase to approximately 1% and 0.3% for the capital cost and CO_2 capture cost respectively, as can be observed in Figure 8. That is why 0.85 cost exponent is adopted for packing height less than the Base case in the IDF Scheme. This is because of the peculiarity of the absorption column and packings in respect of economy scale principle as explained earlier.

In the case of the lean/rich heat exchanger temperature difference iterations, the IDF tool errors for the capital cost and CO_2 capture cost estimates are between -0.66 to 0.18% and -0.30 to 0.16%.

These are very small errors and are acceptable. They do not have any effect on cost optimization calculations or sensitivity analysis results when process parameters are varied several times. Therefore, the IDF tool is suitable for quick and accurate cost estimation and other economic analysis of solvent-based CO_2 capture processes involving several iterations of the entire process from simulation to cost estimation.

4 Conclusion

A simple scheme was developed in Aspen HYSYS for quick and accurate iterative process simulations, equipment dimensioning and cost estimation of a CO_2 capture process. We refer to it as the Iterative Detailed Factor (IDF) Scheme. It is implemented by the aid of the Aspen HYSYS spreadsheet's function. It was validated in this work. The average error in all the iterations is 0.2% of the reference cases. The cost optimum temperature difference in the lean/rich heat exchanger estimated using the IDF tool with fixed tubesheets shell and tube heat exchangers (FTS-STHX) is 15°C. This agrees with recent literature.

Application of detailed factorial methodology in cost estimation is time-consuming. However, the IDF tool reduces the time required for economic analysis of CO_2 capture processes for subsequent iterations to less than a minute after simulation.

Therefore, with the IDF Scheme, accurate cost optimization of CO_2 capture processes, sensitivity analysis of process parameters and economic assumptions as well as market conditions, solvent and blends cost analysis and other iterative cost studies of CO_2 capture processes can be conducted using detailed factorial method in relatively short time (minutes instead of hours or days).

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