

Demonstrating a Refinery-adapted cluster-integrated strategy to enable full-chain CCUS implementation - REALISE.

D3.8 Open access CO₂ capture tool for refineries- the OCTOPUS tool (manual)

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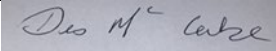
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Executive summary

The OCTOPUS tool (**O**nline **C**alculator **T**o **O**ptimise **C**O₂ capture **P**rocesses for **m**ultiple **S**tacks) is a web based open access application (<https://octopus.sensorlab.tno.nl/>), designed for refineries, chemical clusters or other companies to perform a high-level evaluation of the feasibility of post-combustion CO₂ capture for their processes. The tool is a result of work performed in the Horizon 2020 project REALISE CCUS (<https://realiseccus.eu/>). In this project, TNO and NTNU have collaborated closely to develop this tool.

The tool is designed in such a way that it is user friendly and is able to give high-level design and cost estimations for carbon capture processes within a few clicks, using relevant process data from the user. The tool is additionally able to **evaluate the integration of multiple emission sources into** a single carbon capture process. Integrating CO₂ capture from multiple emission sources can potentially decrease the cost of the overall process and is an interesting option for refineries and chemical clusters to consider in their approach to decarbonise their sites.

Where CO₂ capture simulations require long computational time for simulations and design and costing software normally require a lot of manual effort, this is not the case in the OCTOPUS tool. Using a simulation database instead of actual simulations and combining this with embedded sizing and cost calculations allows case studies to be worked out instantly.

This report serves as a manual for users on how to use and interpret the results of the tool, including a description of the workings of the tool and the main assumptions used in the development of the tool.

Note: The OCTOPUS tool only generates results to assess initial high-level feasibility of carbon capture systems and should only be used as such. Detailed design studies are necessary to assess the actual feasibility specific to the considered process.

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1 How to use the OCTOPUS tool

This chapter serves as an introduction towards users on how to use the tool.

The OCTOPUS tool is a web-based tool that is hosted by TNO and available from web browsers world-wide at: <https://octopus.sensorlab.tno.nl/>. For security reasons, it is required for everyone to request a username and password with TNO for usage of the tool. These credentials will have to be entered when navigating to the website. The web site should be accessible from any modern web browser, although smaller screens may be less suitable to display all the input fields. Any technical problems in reaching the tool can be reported by sending an e-mail to one of the TNO authors of this manual.

The tool does not log any information that is entered by the user and the results are also not saved anywhere.

1.1 User input

The main input of the tool coming from the user is the information on the flue gases to be handled by the CO₂ capture process. The tool allows input of several flue gas parameters such as: flow rate, temperature of the flue gas, pressure of the flue gas stream and CO₂, O₂ and H₂O concentrations in the flue gas. The user can select a single stack if calculations are performed for a site with only one emission source, or the user can select up to 5 stacks to perform calculations for multiple stacks at the same time. Additionally, the solvent to be considered and the target CO₂ capture rate can be selected at this stage. In the current version of the tool, the first-generation MEA solvent and second-generation HS3 solvent are included. For MEA, 90%, 95% and 99% target capture rates are included, while for HS3, only the 90% target capture rate is included.

Stack 1	Stack 2	Stack 3	Stack 4	Stack 5
Flue gas flow rate (Nm ³ /hr) 100000	Flue gas flow rate (Nm ³ /hr) 100000	Flue gas flow rate (Nm ³ /hr) 100000	Flue gas flow rate (Nm ³ /hr) 100000	Flue gas flow rate (Nm ³ /hr) 100000
Temperature (°C) 100	Temperature (°C) 100	Temperature (°C) 100	Temperature (°C) 100	Temperature (°C) 100
Pressure (mbarg) (0 = at...) 0	Pressure (mbarg) (0 = at...) 0	Pressure (mbarg) (0 = at...) 0	Pressure (mbarg) (0 = at...) 0	Pressure (mbarg) (0 = at...) 0
CO ₂ concentration (vol% ...) 10	CO ₂ concentration (vol% ...) 10	CO ₂ concentration (vol% ...) 10	CO ₂ concentration (vol% ...) 10	CO ₂ concentration (vol% ...) 10
O ₂ concentration (vol% dry) 8	O ₂ concentration (vol% dry) 8	O ₂ concentration (vol% dry) 8	O ₂ concentration (vol% dry) 8	O ₂ concentration (vol% dry) 8
H ₂ O concentration (vol%) 8	H ₂ O concentration (vol%) 8	H ₂ O concentration (vol%) 8	H ₂ O concentration (vol%) 8	H ₂ O concentration (vol%) 8

+ ADD STACK - REMOVE STACK

Solvent Type	Target CO ₂ Capture Rate
Solvent type MEA	Target CO ₂ capture rate 90%

Figure 1, user input regarding flue gas and selection of solvent type and target CO₂ capture rate

With the user input completed, integration options can be selected as preferred by the user. The integration options included in the tool are shown in Figure 2. It is possible to integrate the raw flue gases before the quench, to allow for complete centralised CO₂ capture systems, saving a lot of equipment and CAPEX in the process. When flue gas integration is not possible, for instance, because of safety issues or distances between stacks, it can be considered to integrate the rich solvent streams with each other, as combining rich solvents seems to pose less safety risks and is expected to be cheaper than transporting flue gases over long distances. In this case, each stack still needs its own quench and absorber system, but the rest of the capture system can be integrated into a single process. Alternatively, the gaseous CO₂ product can be integrated, which then allows for a centralised compression station, but all other equipment is designed per stack. Lastly, the CO₂ can be integrated after the compression station. Choosing this option means no integration in the OCTOPUS tool is done, as the outlet boundary condition of the tool is chosen at the exit of the compressed CO₂ stream at 20 bara.

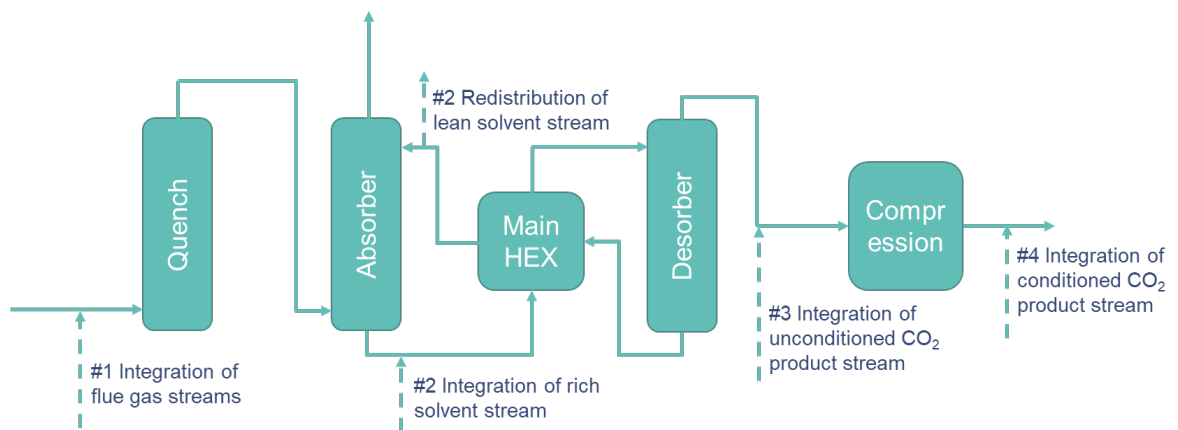


Figure 2, integration options for CO₂ capture systems.

The implementation of these integration options in the OCTOPUS tool is shown in Figure 3 for a case where the user has selected five stacks to integrate. In the example, the user selects to combine the flue gases from stacks 1 and 2, resulting in the combination F12. The user also decides to integrate the solvent of F12 and F3, creating integration SF12F3. The user additionally decides to integrate the unconditioned CO₂ product of stack SF12F3 and SF4, creating the combination CSF12F3SF4. The user additionally decides to have no integration options for the fifth stack, which is consequently called CSF5. The final result gives information on the total cost of the integrated solution with stacks 1, 2, 3 and 4, but will also provide information on important individual sizing and costing of relevant equipment, such as the absorber sizing and cost for stack 3, which is only integrated after the absorber with the rich solvent streams.

This approach allows the user to select any type of integration they want to analyse, and to quickly generate results for all kinds of integration options they prefer. It is also possible to select no integration options, and analyse a standalone capture system, as was done in the previous example with stack 5.

It is important to note that the tool currently does not calculate the cost of transporting fluids (flue gas, solvent or CO₂ product) over a certain distance, which could have an effect on the business case. For instance, it can be expensive to transport flue gases over long distances. This must be taken into account when using the tool with the integration options.

+ Flue Gas Flow Integration

This component allows you to integrate Flue Gas Flows.

1
 2
 3
 4
 5

F12
 F3
 F4
 F5

SF12F3
 SF4
 SF5

+ Solvent Flow Integration

This component allows you to integrate Solvent Flows.

1
 2
 3
 4
 5

F12
 F3
 F4
 F5

SF12F3
 SF4
 SF5

+ Unconditioned CO2 Flow Integration

This component allows you to integrate Unconditioned CO2 Flows.

1
 2
 3
 4
 5

F12
 F3
 F4
 F5

SF12F3
 SF4
 SF5

Figure 3, integration options as included in the OCTOPUS tool.

With the integration options selected, the user can input relevant utility cost parameters regarding steam, electricity and cooling water, as shown in Figure 4. For cooling water, these costs are defined as the cost of cooling water make-up in evaporating cooling systems, which is dependent on the amount of cooling required by the capture system. Additionally, default financial parameters can be used, or the user can choose to enter their own parameters that can affect CAPEX and Fixed OPEX calculations.

The optimisation target for the tool can be either selected as energy or CAPEX. To have the option to optimise for CAPEX is unique and is generally not found in techno-economic analysis (TEA) of CO₂ capture systems, as often designs are optimised for energy in the simulation phase of a techno-economic analysis.

Utilities

Utility Prices

Steam price (€/GJ)
4

Electricity price (€/MWh)
50

Cooling water price (€/m³)
0.1

Financial Parameters

Financial parameters can be customised.

Use default financial parameters

Optimisation Target

Optimisation target determines the parameter of focus, either energy (heat duty) or CAPEX.

Optimisation target
Energy ▼

Figure 4, input regarding utilities, financial parameters and optimisation target.

1.2 Result generation

When the user clicks the “Generate results” button, the calculations are performed almost instantly, and the main results are returned to the user. Figure 5 shows the overall cost of CO₂ capture for five non-integrated stacks with flue gas flow rates ranging linearly from 100000 Nm³/hr to 500000 Nm³/hr. The effect of scale on decreasing specific costs for CO₂ capture is clearly shown by the graph and gives indications of how this tool can be used to evaluate several case studies.

Note that solutions that overlap are hard to distinguish visually in the plot, and you might see a single dot, where multiple solutions overlap. This can be checked by clicking the legend below the graph to toggle the individual solutions’ visibility.

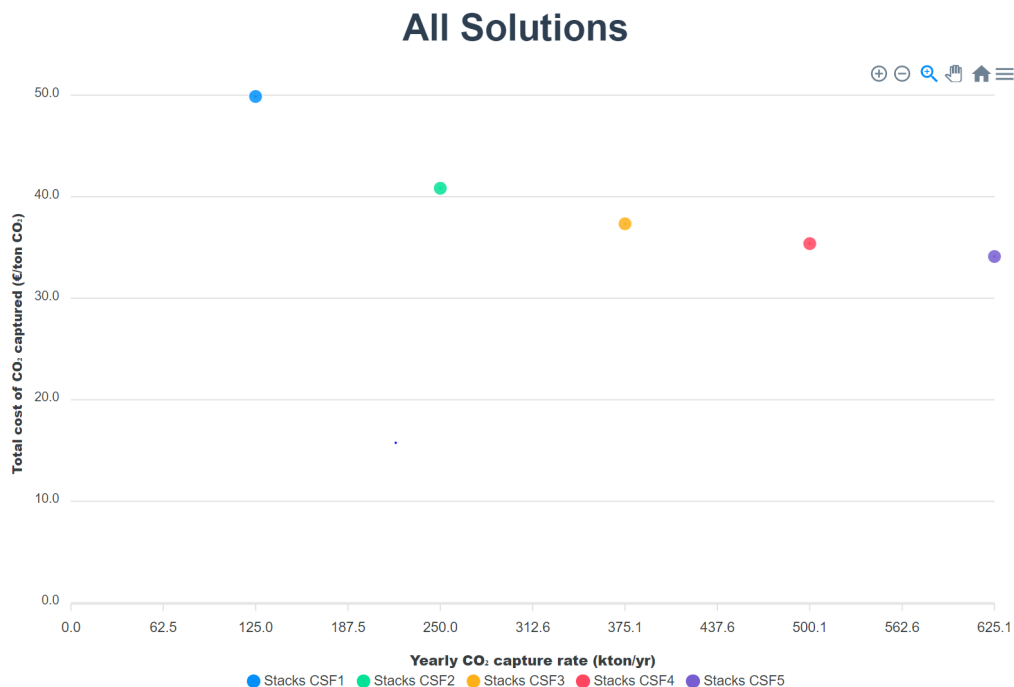


Figure 5, overall cost of CO₂ capture for all (integrated) solutions.

More specific results for the cases studied by the user are found in tables below the overall cost of CO₂ capture plot and includes information on sizing, utility demands and CAPEX of relevant equipment as shown in Figure 6. The user can use this data to

calculate different cases and compare the results of integration options to assess the feasibility of different process configurations for their site.

Flue gas specific results										
Flow ID	CO ₂ capture rate (kg/h)	Absorber diameter (m)	Absorber packing height (m)	Absorber total height (m)	Absorber Packing Capex (MEUR)	Absorber Shell Capex (MEUR)				
1	15857.92	4.49	17	33.76	2.51	3.36				
Solvent specific results										
Flow ID	CO ₂ capture rate (kg/h)	Lean solvent flow rate (kg/h)	Desorber diameter (m)	Desorber packing height (m)	Desorber total height (m)	Reboiler duty (MW _{th})	Specific reboiler duty (MJ/kg CO ₂)			
SF1	15857.92	207616.41	2.67	12	27.37	15.9	3.61			
Gaseous CO₂ product specific results										
Flow ID	CO ₂ capture rate (kg/h)	Compressor 1 electrical duty (kW)	Compressor 1 CAPEX (M€)	Compressor 2 electrical duty (kW)	Compressor 2 CAPEX (M€)					
CSF1	15857.92	458.52	2.87	358.58	2.7					
Overall results										
Flow ID	Total CO ₂ captured (kton/yr)	Total CAPEX (M€)	Electricity demand (MW _e)	Total heat demand (MW _{th})	Cooling water demand (MW _{th})	Solvent costs (€/ton CO ₂)	Specific CAPEX (€/ton CO ₂)	Specific variable OPEX (€/ton CO ₂)	Specific fixed OPEX (€/ton CO ₂)	Total costs (€/ton CO ₂)
CSF1	125.02	22.95	1.17	15.9	16.93	2	18.7	20.51	10.66	49.87

Figure 6, overview of results obtained from a case study with 1 stack.

2 Structure of the OCTOPUS tool

The OCTOPUS tool is structured in three parts: (1) a simulation result database, (2) an engine and (3) a user interface. The function and communication between each part is discussed below.

2.1 Simulation result database

Simulations are the backbone of most TEA analysis performed on CO₂ capture. Running simulations using validated models requires a lot of computational time. Additionally, sizing and costing requires much work. For the OCTOPUS tool, a different approach is taken, where a simulation database is created, that can cover a large range of input data given by the user. This way, the input data from the user of the tool is translated to an existing entry in the simulation result database, and the relevant process data can be accessed easily, without actually having to perform the simulations.

2.1.1 Software used.

To generate the necessary data for the tool, the CO₂SIM software from SINTEF and NTNU is used [1], [2]. Both the MEA and HS3 models in the CO₂SIM software are validated against the Tiller carbon capture pilot data. CO₂SIM can, to this extend, be regarded as a best-in-class software, where the models are extensively validated against good experimental pilot plant data.

2.1.2 General flowsheet

The general flowsheet in CO₂SIM for the simulations performed for the OCTOPUS tool can be found in Figure 7. It can be seen that all major equipment of the capture system is included in the simulations, such as the absorber and desorber columns, heat exchangers and pumps. Note that the upstream quench or downstream compression equipment is not included in the simulations. This is separately simulated/calculated in the OCTOPUS tool and is included in the final result.

For the 99% capture rate MEA case study, the heat generation in the absorber was high, causing equilibrium limitation in the absorber column. For the 99% capture rate MEA case, it was decided to include an intercooler in the middle of the absorber packing (regardless of the packing height selected) to ensure moderate temperatures throughout the absorption column, giving much better absorber performance.

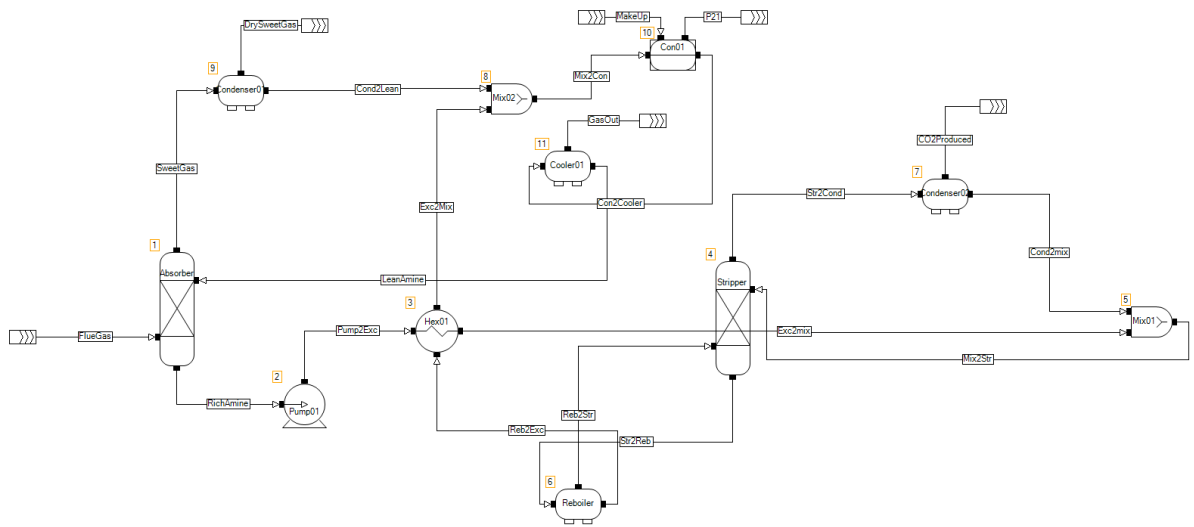


Figure 7, flowsheet used in CO2SIM to generate the data for the simulation database.

2.1.3 Key assumptions in simulations

A set of simulations were performed where for each CO₂ concentration the height of the absorber column and solvent flow rate was varied for various capture rates. This subsection describes some key assumptions during the simulations. The unit names refer to Figure 7.

The input variables for the flue gas are shown in Table 1. It was considered in the simulations that the flue gas had no impurities and the gas was assumed to be saturated with water at 313.15 K.

Table 1, flue gas specifications for the simulations

Variable	Unit	Value
Temperature	K	313.15
Pressure	kPa	101.325
Flow rate	m ³ /h	100,000
CO ₂ molar fraction	-	from 3% to 20% (wet)
H ₂ O molar fraction	-	saturated
N ₂ molar fraction	-	remainder

The input data for the **Lean amine stream** was the temperature (313.15 K for all cases), pressure (101.325 kPa for all cases), the composition (based on solvent type) and flow rate. The H₂O molar fraction was set to satisfy the solvent concentration. The lean loading is a simulation result.

The **absorber column** in CO2SIM requires the specification of the geometric parameters: diameter and packing height. The packing height was varied from 5m to 30m. The diameter was kept constant at a gas velocity of 2 m/s.

Pumps are required in several places in the capture plant, but don't necessarily need to be included in the simulations. The only pump included in the simulations is the rich pump, **Pump1**, to ensure that there is no solvent flashing in the heat exchanger thus to avoid multiphasic flow through the rich/lean heat exchanger. The outlet pressure of this pump was set to 1000 kPa.

Hex01 is the lean/rich heat exchanger and an approach temperature of 10 °C between the inlet of the rich amine and the outlet of the lean amine was defined.

The **desorber column** requires the specification of the geometric parameters. The diameter was fixed as 60% of the absorber diameter and the height was fixed as 12m. The **reboiler** was set as a flash QP, in which the pressure was set to 190 kPa and the reboiler duty value was changed to reach the desired capture rate.

On the top of the absorber, a condenser was used instead of water wash system. This was done to reduce the computational time and to keep the water balance closed in the simulations. The **condenser01** was simulated with a flash PT unit- The pressure was set to 101,325 kPa and the temperature 313.15K. On the top of the stripper, a condenser recovers the water from the stripper outlet. This condenser, **condenser02**, was set as a flash PT, the pressure value was set as 190 kPa and the temperature was 313.15K.

A solvent make-up unit is needed in simulations to replace the solvent and water losses from the process to allow the simulation to converge to a stable solution. In CO2SIM, this unit is represented by the unit called "CON1". This unit requires the specification of the desired amine molar fraction, the lean amine flow rate and temperature. This unit was set to keep the solvent concentrations (both for MEA and HS3) and a temperature of 313.15K.

The lean solvent stream must be cooled before it enters the absorber column. The lean cooler, **Cooler01**, reduces the lean solvent temperature to 313.15K.

For the cases with 99% capture rate using the MEA solvent, an **intercooling stage** in the middle of the absorber packing is included, cooling the solvent to 313.15K and injecting it back on the same height.

2.1.4 Populating the database

To populate the simulation database to be used in the OCTOPUS tool, several parameters are varied between simulations, which are summarised in Table . Working out the matrix with all variables, more than 10000 simulations are summarised in the database. Covering this wide range of CO₂ concentrations allows the OCTOPUS tool to cover a large part of the flue gases available in an industry where post-combustion carbon capture with amines can serve as a feasible solution. Allowing the user to select the capture rate helps put higher capture rates into perspective compared to the historical 90% capture.

Note that flow rate is not a parameter that is varied in the simulations, while flue gas flow rates vary widely in industry. This is because the size variable can be covered by scaling the results for a specific solution (absorber diameter, heat demands, mass flows) with the ratio of the actual flue gas flow rate over the flue gas flow considered in the simulation. It is assessed per parameter how they scale with size. This, for instance, means that the solvent flow rate is scaled linearly with flue gas flow rate, while the

absorber diameter scales with the square root of the flue gas flow rate. Taking this approach, any simulation result can be translated to any size given as input by the user.

Table 2, overview of variables covered by the simulation database.

Parameter	Unit	Range	Number of steps
CO ₂ capture rate	%	90, 95, 99	3
CO ₂ concentrations	vol%	3 to 20	18
Packing height	meter	7 to 30	24
Solvent flow rates	kg/hr	Around optimum L/G	4 to 10

2.1.5 Main results from simulations

The specific reboiler duty (SRD) of a typical L/G optimisation result from a single CO₂ capture rate, CO₂ concentration and packing height is shown in Figure 8. The often-observed U-shaped optimisation curve is present, which shows that an optimum solvent flow rate exists for the specific conditions. This curve is observed for most of the capture rates and packing height considered in the simulation database, showing the consistency of the database.

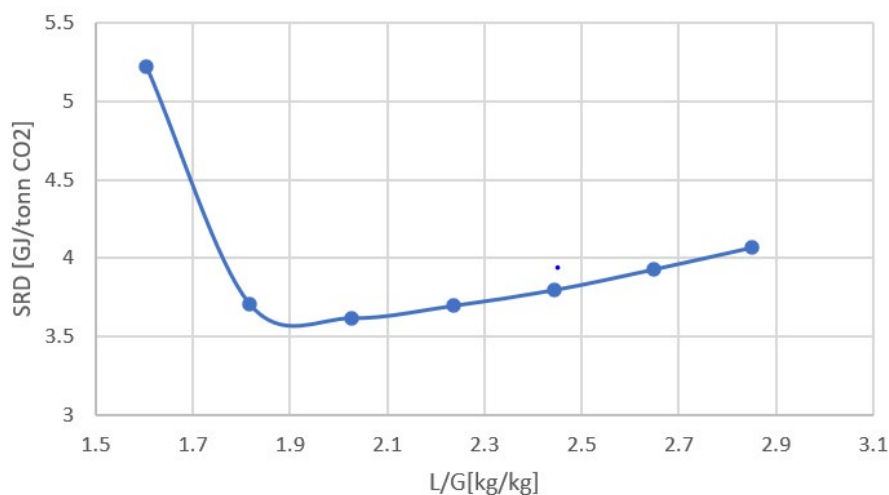


Figure 8, L/G optimisation curve for 95% capture, 10% CO₂ concentration and 25 meters of packing height for MEA.

The minimum SRD obtained for each packing height for 90% capture, the HS3 solvent and three different CO₂ concentrations is shown in Figure 9. The effect of the packing height on the minimum reboiler duty is clearly observed, showing which packing height must be considered to get good CO₂ capture performance. Also, the effect of CO₂ concentration in the flue gas is shown, where higher CO₂ concentrations require lower packing heights to have good energy performance of the system.

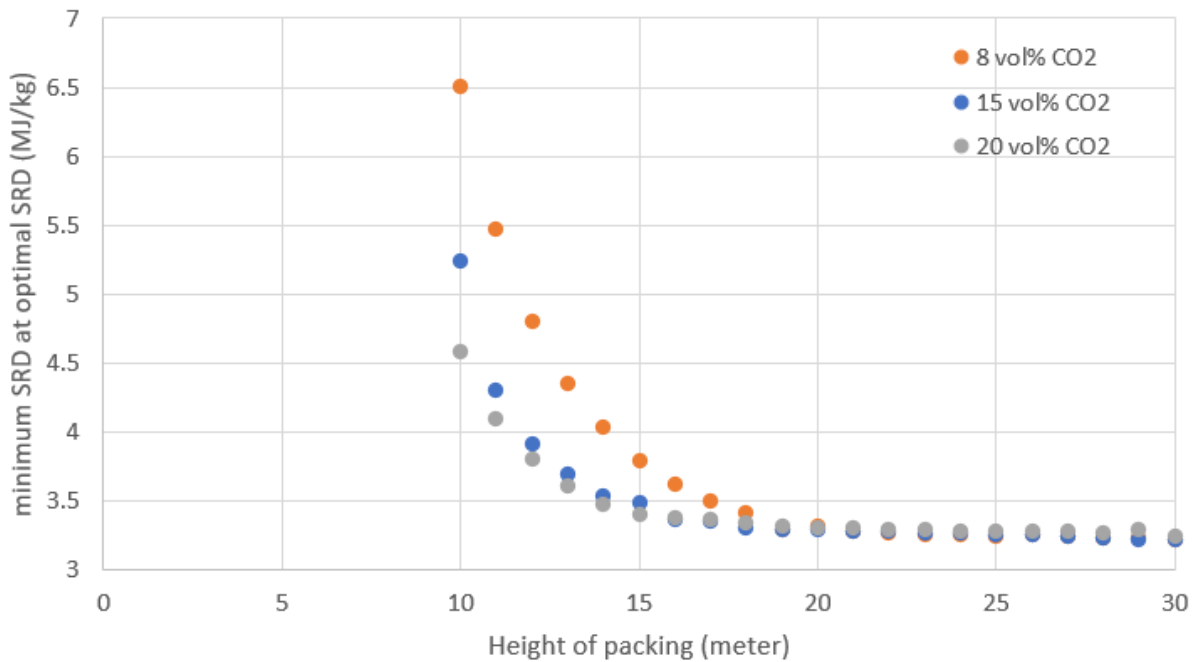


Figure 9, minimum SRD at every packing height, calculated for three different CO₂ concentrations using 90% capture with the HS3 solvent.

Because an intercooler was only applied to the 99% capture rate simulations using MEA, it is possible that this option gives lower reboiler duty values than the 90% or 95% capture rate data for MEA in specific cases. This is important to keep in mind while performing analysis with different capture rates in the tool.

2.2 The OCTOPUS Tool User interface

The user interface (UI) is the part of the tool visible for the user. The UI is hosted at the following web address: <https://octopus.sensorlab.tno.nl>. At this location, the user can input all relevant information on their process, like flue gas specific information, energy costs and cost calculation variables as explained above. Once the input is completed, the tool will send a query with all relevant information to the engine, that will process the query and perform calculations on the data. Results are returned to the user interface almost instantly.

2.3 Engine

The engine is the heart of the tool, where the main calculations on the simulation data are performed. This section gives an overview of the functions of the engine.

2.3.1 Energy and CAPEX optimisation route

As stated above, the OCTOPUS tool can both optimise the results for energy and CAPEX. Figure 11 below graphically shows the methodology that is used for this. Since the OCTOPUS tool considers very high packing heights (up to 30 meters), this highest packing height can be considered as the packing height with the lowest SRD for that

specific CO₂ concentration. A multiplication factor is applied to this minimum SRD and the packing height corresponding closest to that SRD is selected. The multiplication factor is dependent on the optimisation method selected. If energy is selected as optimisation target, 2% is added to the minimum SRD, and the packing height closest to the new SRD is selected. The rationale behind this is that this can represent an efficient packing height to optimise for energy, as increasing the packing height further does not yield a much further decrease in SRD. When CAPEX is selected as the optimisation target, 30% is added to the minimum SRD, and the packing height closest to this new SRD is selected. The rationale behind this is that a 30% higher SRD than the minimum SRD is considered high, but requires much lower packing heights. If CAPEX is dominating the total capture costs (for instance for small scale systems), this approach could yield lower total capture costs.

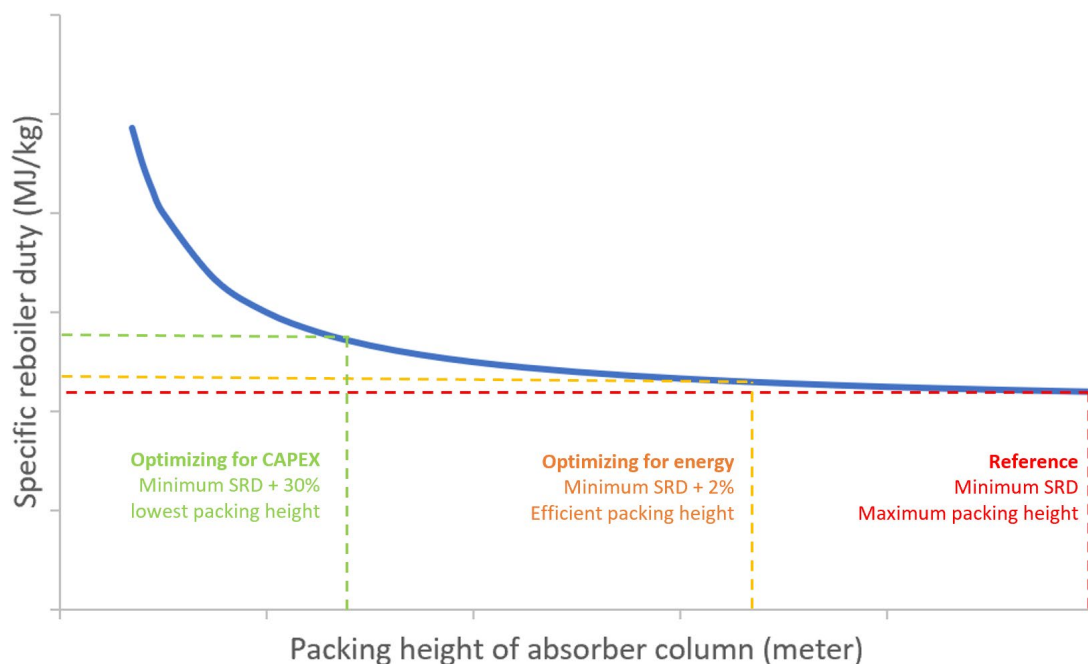


Figure 10, graphical representation of the energy and CAPEX optimisation methods, as included in the OCTOPUS tool

2.3.2 Searching for the closest solution in the database

With all input completed from the user, the UI sends the relevant parameters. This information is used in the engine to access the simulation database using several variables that determine which simulation to retrieve the data from. The important variables that are used to search for the right simulation in the database are listed below.

- Type of solvent → MEA and HS3 for this version of the tool
- Capture rate → 90%, 95% and 99% for MEA and 90% for HS3
- CO₂ concentration in flue gas → Given by user (can change during calculation because of H₂O condensation in quench)

With these variables and the chosen optimisation target, two other variables are determined, that specify the specific solution that will be used for further calculations. These variables are:

- Packing height → Resulting from the optimisation case

- L/G ratio → The simulation with the L/G ratio giving the lowest SRD is chosen

With all these variables determined, a single simulation result can be selected that is returned to the engine for further calculations.

2.3.3 Scaling solution to the right flow rate

As stated above, the simulations are only performed for a reference size. All information from the selected simulation file is transformed to the size defined by the user. The flue gas flow rate ratio (between user data and reference case) is used as the sizing factor to scale up any variables. This scaling is divided into three categories:

- Linearly scaled variables: Flow rates, heat exchanger duties etc.
- Square root scaled variables: Column diameters
- Non-scaled variables: Temperatures, CO₂ loading in the solvent etc.

Using this approach, all variables are scaled, and the final results are generated.

2.3.4 Calculations on quench and CO₂ product compression

As is shown in Figure 7, the simulation database does not cover a quench column or CO₂ compression station. Both the quench and compression station are calculated outside of the tool.

The quench is assumed to have a diameter which is identical to the absorber column and has a four meter packing height. The cooling duty required for the quench system is calculated using the temperature and water content of the incoming flue gases specified by the user. With this information, all relevant equipment around the quench can be calculated. In the current version of the tool, it is only possible to consider flue gases that have a water concentration above the saturation concentration at 40 °C, so that there is always condensation in the quench.

For the compression station, the only relevant input is the amount of CO₂ to be compressed. Compression towards 20 bara is assumed in a two-stage isentropic compression system with intermediate cooling, for which the relevant calculations are included in the tool.

2.3.5 Applying integration options to the query

When integration options are added to the query by the user, the engine calculations are impacted. How these calculations alter is dependent on the integration option selected. For flue gas integration, the flue gas streams are simply combined, and a new flue gas flow rate with a new composition is calculated. For the gaseous CO₂ product integration, the CO₂ product streams are simply combined, generating a new larger CO₂ product stream.

Solvent integration, is more difficult, as the integration is performed within the simulations obtained from the simulation database. The OCTOPUS tool uses a relatively simple method. First, the selected simulation data from the database for each stack separately are extracted from the database. The rich solvent streams are combined, and a new combined rich solvent flow rate and CO₂ loading is calculated. Then, the lean loading is selected from the stack with the highest amount of CO₂ in the flue gas. The simulation database is then again consulted to find the simulation that is closest to the lean and rich loadings obtained from this exercise. The resulting simulation data for the equipment

downstream of the absorber is scaled using the new rich flow rate. Note that this is not the perfect way to perform solvent integration, but it should be sufficiently accurate for the purpose of the OCTOPUS tool.

3 Assumptions in tool

The important assumptions used in the calculations and cost estimation of the tool are summarised in this section to increase the transparency on the working of the tool, and to put the final results obtained in perspective.

3.1 Model assumptions and constants

The main assumptions that are used in the tool to perform calculations on the obtained simulations data is shown in Table .

Table 3, main simulation and design assumptions in the OCTOPUS tool.

Variable	Unit	Value
Flue gas density	kg/m ³	1.1
Heat capacity flue gas	kJ/kg-K	1.0
Heat capacity of water	kJ/kg-K	4.186
Heat of vaporisation of water at 40 °C	kJ/kg	2406
Pressure of flue gas after blower	bara	1.05
Stripper pressure (and CO ₂ product pressure)	bara	1.9
Pressure of CO ₂ product after first compressor	bara	7.0
Pressure of CO ₂ product after second compressor	bara	20.0
Packing height quench	meter	4
Cooling water inlet temperature	°C	20
Cooling water outlet temperature	°C	30
Steam temperature for reboiler	°C	135
Heat transfer coefficient liquid-liquid HEX	W/m ² -K	2000
Heat transfer coefficient condensing gas-liquid HEX	W/m ² -K	500
Specific heat ratio CO ₂	[-]	1.28
Pressure loss vertical transport of water	bar/meter	0.1
Pressure drop of pumping liquids through heat exchangers	bar	0.5
Cooling water make-up rate	m ³ /GJ	1
Efficiency of blower	%	85
Efficiency of pumps	%	80
Efficiency of compressors	%	85
Thickness of column shell	mm	12
Density of stainless steel	kg/m ³	7500

3.2 Costing assumptions

The costing of the equipment is performed using the methodology described by Towler and Sinnott [3]. This chemical engineering design book has been chosen as the reference for the OCTOPUS tool, as it allows for cost calculations of all equipment relevant to CO₂ capture using only publicly available data. Since the book used 2010 USD as the cost basis, this has been updated to 2020 costs using the Chemical Engineering Plant Cost Index (CEPCI). Additionally, since the Towler and Sinnott book only gives equipment costs, these have to be translated to total installed costs. To do this, the Enhanced Detailed Factor (EDF) method has been applied, which is able to transform equipment costs into installed costs per equipment [4]. The EDF methodology

has been condensed for the purpose of the OCTOPUS tool to a simple correlation that links the equipment costs and the installation factor as shown in Figure 12. Additionally, a custom cost curve using a lower pre exponential factor of 10 is generated for compressors, as compressors are generally expensive pieces of equipment that have lower installation factors than other equipment as they are often more modular than for instance large absorption towers.

Additionally, for the calculation of annualised CAPEX, the annuity factor method is used, which is shown in Figure 13 and uses the lifetime and the plant and the cost of capital to account for depreciation effects. The total CAPEX is divided by the annuity factor to calculate the annualised CAPEX. Further assumptions in the cost calculations are shown in Table .

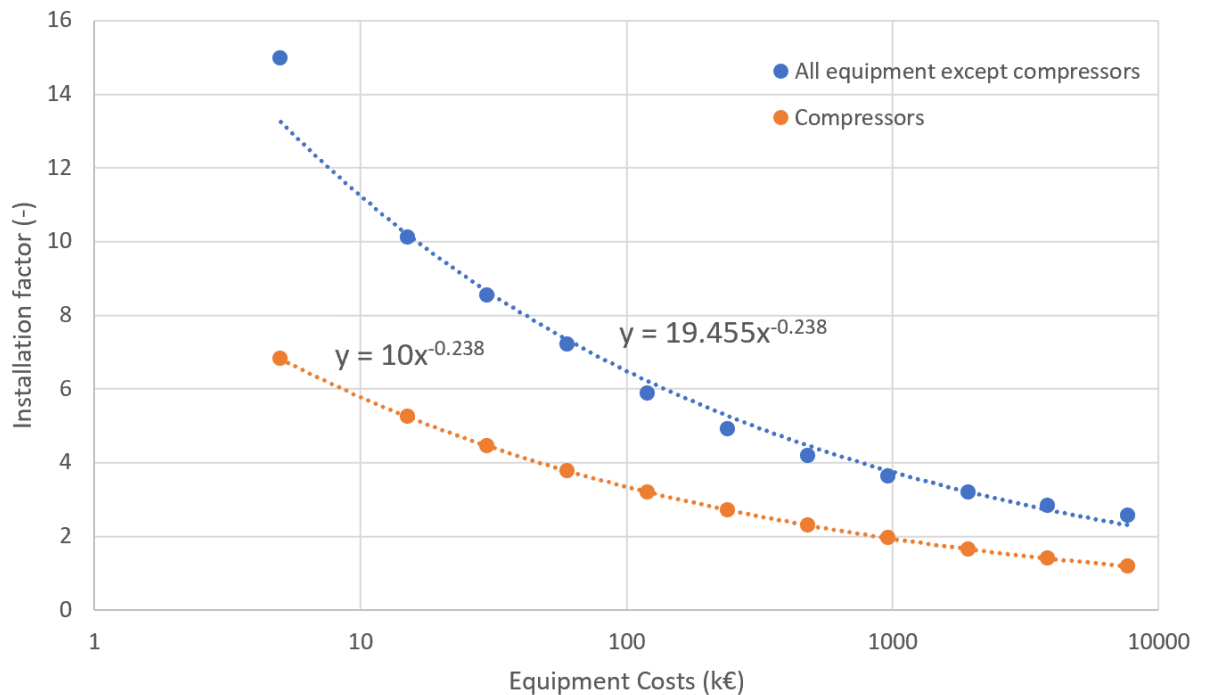


Figure 11, The installation factor as a function of the equipment costs, with data obtained from [4], and the custom installation factor curve for compressors.

$$\text{Annuity Factor} = \frac{1 - \frac{1}{(1+r)^t}}{r}$$

where:

r = Cost of capital

t = Number of periods

Figure 12, annuity factor method

Table 4, main cost calculation assumptions in the OCTOPUS tool

Variable	Unit	Value
Dollar to Euro exchange rate (01/04/2020)	\$/€	0.91
CEPCI 2010		532.9
CEPCI 2020		596.2
Availability factor of process	%	90
Number of operators needed	[-]	6
Number of technologists needed	[-]	1
Cost of operator	€/year	60000
Technologist costs	€/year	100000
<u>Default financial parameters in UI of tool</u>		
Maintenance costs	yearly% of TPC*	2.5
Insurance costs	yearly% of TPC*	1
Yearly overhead and administrative costs	yearly% of TPC*	0.3
Lifetime of plant	years	20
Discount factor	[-]	8

*TPC = Total process costs

3.3 Solvent costs

Solvent costs are included with simple correlations in the current version of the tool. The price of MEA and HS3 used are 3.4 €/kg and 51 €/kg respectively, based on best price estimates in the REALISE project by the consortium members. Solvent make-up rates of 1.43 kg/ton CO₂ and 0.53 kg/ton CO₂ are used for MEA and HS3 respectively, based on estimates from Tiller pilot plant campaigns (SINTEF). These values are used consistently throughout the REALISE project. A future version of the tool should include more detailed calculations on solvent losses, to make this aspect more accurate.

4 Recommendations for further development of the OCTOPUS tool

Several recommendations are given for further development of the OCTOPUS tool:

- Further extension and validation of the simulation database used in the OCTOPUS tool should be done. An example of this is applying intercoolers to the 90% and 95% capture rate cases, as this seems to result in lower reboiler duties. This way, also more detailed energy comparison studies can be performed between results of different capture rates.
- Simulations should be performed with a fixed flooding percentage on the stripper side. This way, the stripper diameter would scale with the CO₂ concentration in the flue gas, which creates a more realistic scenario.
- The current integration options do not include the cost of transporting the different fluids to other part of the process. Integrating a methodology to include this could give users of the tool further insights into the potential of integrating CO₂ capture systems.
- The UI could be extended with options for its users to add constraints. This way, based on, for example, the utility or plot space availability of the company considered, the most optimal solutions can be found.
- The CAPEX estimations in this version of the tool are based on relatively old correlations. Combined with the applied EDF method, this makes compression more expensive than expected. The compression installation factor has already been reduced to mitigate this effect. However, still more updated and more detailed CAPEX estimates could help further increase the tool's accuracy.
- Solvent costs are taken into account in the tool only with simple factors. Integrating more detailed calculations and models on solvent emissions, degradation, treatment and replacement rates could help further evaluating the effect of many parameters on solvent losses and cost of CO₂ capture in general.
- CESAR1 is a well-tested second generation open access solvent that shows clear benefits over the first generation MEA solvent in terms of energy demand and solvent stability. Implementing this solvent into the tool would be beneficial to assess the potential of other second generation solvents.
- The SRD multiplication factor defined as 2% and 30% for Energy and CAPEX optimisation respectively are fixed in the current version of the tool. Giving users flexibility to define their own multiplication factor would give the user even more freedom to optimise their case studies with the tool.

5 References

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