The OCTOPUS tool (REALISE project)



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REALISE-CCUS project





Demonstration of a refinery-adapted cluster-integrated strategy to enable full-chain CCUS implementaion - REALISE

- □ Project period: 05.2020 10.2023
- **Project partners:**
 - 14 EU partners
 - 2 partners in China
 - 1 partner in S. Korea
- □ *Project budget:* €7,131,752

Funded by the European Unition's Horizon Europe Research and Innovation Program (Horizon Europe (europa.eu))



The REALISE story



A highlight of the REALISE project



ireland-refinery-whitegate-1.3754690

Tiller CO₂ pilot \rightarrow SINTEF

- CO₂ liquefaction prototype
- Energy and emissions measurements

How to integrate and optimize carbon capture from multiple sources?



The OCTOPUS tool



Structure of the OCTOPUS tool

User interface (web app)

User can supply general info, stack data, constraints and optimization objectives to tool





Engine

Engine takes the data from the user interface, and matches this with the right data from the database

Engine performs calculations on all possible configurations, using given constraints and the optimization objective

Simulation database

A CO₂ capture simulation database has been created using the CO2SIM software

In the CO2SIM program, many simulations are performed while varying: (1) Capture rate, (2) CO₂ concentration, (3) absorber packing height, (4) liquid flow rate

Note: By using this approach, results are generated instantaneous by the OCTOPUS tool

Creating simulation result database

The CO₂ capture flowsheet in CO2SIM



The database is created from simulation results

		D			E		Ci Ci				- N		191	14		. E 2	- Q
		03002_10m_90cap_L0	03CO2_10m_90cap_L	03CO2_10m_90cap_L(03CO2_10m_90cap_L0	03CO2_10m_90cap_L(03CD2_10m_90cap_L0	308									
Absorber																	
Packing heigh	nt [m]	10	10	10	10	10	10						SRD	vs LG			
Column diame	eter (m)	4.2	4.2	4.2	4.2	4.2	4.2										
Flue Gas										80							
Flue gas flow r	rate (Nm3ih)	87555.97698	87555.97698	87555.97698	87555.97698	87555.97698	87555.97698			25							
Flue gas flow r	rate (m3ih)	100061.7026	100061.7026	100061.7026	100061.7026	100061.7026	100061.7026										
Flue gas flow r	rate (kmolih)	3894	3894	3894	3894	3894	3894			20	\rightarrow						
Flue gas Temp	p. [C]	40	40	40	40	40	40										
Flue gas Press	s[kPa]	101.325	101.325	101.325	101.325	101.325	101.325			15							
CO2 at inlet (m	nol / wet)	3	3	3	3	3	3										
H2O at inlet (m	nol%vet)	7.26	7.26	7.26	7.26	7.26	7.26			10							
Soluent												· ·					
Soluent erel	flow rote (kaliw)	197759 8692	175510.0508	153208.0566	130842 5997	108414 3209	85907 7098			- 5 -							
Solvent Lean	flow rate (kgn1)	8280	7360	6440	5520	4600	3680										
Solvent Lean	Townale (kinoinii)	0200	1300	0440	3320	4000	3000			0.7		1.9	1.1	1.3	1.5	1.7	1.9
Clinit	cool it	0.004040570	0.0100720000	0 104001700	0.40000000	0 40000000	0.05*040000										
SolventLean	CO2 loading	0.224010573	0.212573032	0.134331700	0.100030043	0.123405363	0.051040036										
Hich Amine		11.007.000	10.05004740	10 50345400	10 00070040	10.00011070	10.05430400										
Solvent High I	lemp. [L]	44.22745133	43.85301719	43.53715126	43.28270216	43.08814278	42.951/9108						lean loa	ding ve	16		
Solvent Hich U	JU2 loading	0.330796681	0.332028893	0.33097527	0.325957783	0.314482917	0.29041686						icuit iou	ung va	10		
CU2 product										0.25							
CO2 recovery	(%)	0.90005339	0.900014928	0.899998108	0.899982845	0.899942699	0.899917283									-	-
CO2 Captured	d (kg/h)	4627.389449	4627.192704	4627.106282	4627.027941	4626.822275	4626.692165			0.2					-	•	
L_G Ratio		1.828970277	1.623194168	1.416917016	1.210089928	1.002663338	0.794512296							_			
Stripper										0.15			-				
Packing heigh	nt [m]	12	12	12	12	12	12					~					
Column diame	eter [m]	2.5	2.5	2.5	2.5	2.5	2.5			0.1							
Reboiler										0.1		/					
Rebailer Press	sure [kPa]	190	190	190	190	190	190										
Reboiler Term	perature [C]	119 7698968	120 1550469	120 6702189	121 315274	122 0255038	122 5682155			0.05							
Robeiler Dutul	IL UL1	28527908.33	27991062.7	27993694.46	29194744.21	36962570.93	119067604.9										
Specific Poly	der dutu IG Broon CD	20021000.00	E 047092596	E 026160361	6 309610527	7 967146496	25 51979413			0							
Candidate	ner dag (outonin co	0.100011010	0.041032300	0.020100301	0.000010321	1.301140400	20.01010410				12	0.9	1.1	1.3	1.5	1.7	1.9
Condenser		40	40	40	40	40	40										
Condenser re	inperature (C)	40	100 0070500	100.0077010	100 5005170	10 4004000	40										
Tempeature I	op ompper [U]	100.4033623	100.0013531	100.3355010	103.5005176	110.4004003	112.3700520						rich loa	ding yr	16		
Cooling Lema	ina	-3216.305336	-3303.020432	-3074.01014	-4170.300107	-0044.720000	-23550.37100						incir iou	ung 15			
Lean Rich Exc	ohanger									0.335							
hexrichtempin	1	44.22745133	43.85301719	43.53715126	43.28270216	43.08814278	42.951/9108			0.33				-	-		
hexrichtempor	ut	108.821867	109.1422699	109.5761646	110.1149637	110.6794607	111.0104588			0.325			~				
hexleantempir	n	119.7698968	120.1550469	120.6702189	121.315274	122.0255038	122.5682155			0.32			/				
hexleantempo	out	54.22745133	53.85301719	53.53715126	53.28270216	53.08814278	52.95179108			0.315			/				
Lean Rich Exh	n Duty	-13384.90287	-12006.45063	-10607.9718	-9184.249401	-7723.705254	-6205.991958			0.11							
Lean Cooler										0.705							
Cooling Dema	nd	1467.91649	-2122.944123	-1536.300078	3041,749344	-277.7385757	475.8184174			0.303							
tempin		54.08619815	53.67883418	53.32495074	53.02353205	52,76624143	52.53796385			0.3		/					
tempout		40	40	40	40	40	40			0.2.95	/						
Rich Purne										0.29							
Pump program	e [kPa]	1000	1000	1000	1000	1000	1000			0.285							
Pump Wesh fly	UL1	229910 9614	212974 1294	196022 0947	159044 996	122025 6669	104941 6744				0.7	0.9	1.1	1.3	1.5	1.7	1.9
r unp work (k	oing	233310.3014	212014.1204	100020.0041	10,000	102023.0000	1010110144										
LeaDe el-M		10.94902997	11 01277701	11 09405422	11 20021022	11 24604216	10 H EE 776003										
noomnonin	20	10.34602367	11.01277701	11.03405432	11.20031032	11.34604316	11.55775003										
ratiopn2o_pci	o/Dottom	10.53655074	12.30307648	15.63954475	23.4794355	51.04081781	422.4066455										
ratioph2o_pci	oZAbs I op	26.12241571	26.14130777	26.1581326	26.17052901	26.17327035	26.17773316										
	RaceCaceN4E	A 02CO2 9m 00con	RaceCaceb4EA	02CO2 0m 00con	BaroCaroMEA 0	3CO2 10m 90cm	RaceCaceMEA 0	2002 11	m 00cor		acoCor		æ		41		
	DaseCaseIVIE/	w_oscos_am_aocab	DasecaseIVIEA_	inacrosTatuTancab	DasecaseiviEA_U	SCO2_1011_90cap	baseCaSeIVIEA_0	5002_11	uu-aocab	6	aseCas	eivicA_U			4		

Number of simulations for populating the database

Parameter	Range	Number of settings
Solvent type	MEA and HS3	2
CO ₂ capture rate	90% and 95%	2
CO ₂ concentration in flue gas	3 to 20%	18
Absorber packing height	7 to 30 meter	24
Liquid flow rates	Around optimal L/G	4 to 10

The total number of simulation results included in the tool is ~15000



Integration of capture processes in clusters



Demonstration of the tool – Stack selection

Single stack query

	⊯ Stack 1
10	Flue gas flow rate (Nm³/hr) 0000
ו 10	Temperature (°C) O
0	Pressure (mbarg) (0 = atmospheric)
10	CO ₂ concentration (vol% dry)
8	O2 concentration (vol% dry)
8	H:O concentration (vol%)

Multi stack query i Stack 1 i Stack 2 i Stack 3 i Stack 4 i Stack 5

Flue gas flow rate (Nm³/hr) 100000	Flue gas flow rate (Nm³/hr) 200000	Flue gas flow rate (Nm³/hr) 300000	Flue gas flow rate (Nm³/hr) 400000	Flue gas flow rate (Nm³/hr) 500000
Temperature (°C) 100	Temperature (°C) 100	Temperature (°C) 100	Temperature (°C) 100	Temperature (°C) 100
Pressure (mbarg) (0 = at	Pressure (mbarg) (0 = at 0	Pressure (mbarg) (0 = at	Pressure (mbarg) (0 = at 0	Pressure (mbarg) (0 = at 0
CO ₂ concentration (vol% 10	. CO₂ concentration (vol% 10	CO2 concentration (vol%	CO2 concentration (vol%	CO ₂ concentration (vol% 10
O2 concentration (vol% dry	02 concentration (vol% dry)	O2 concentration (vol% dry)	O2 concentration (vol% dry)	O2 concentration (vol% dry)
H ₂ O concentration (vol%)	H ₂ O concentration (vol%) 8	H ₂ O concentration (vol%) 8	H ₂ O concentration (vol%)	H ₂ O concentration (vol%)

Demonstration of the tool – Integration option selection



Demonstration of the tool – Utilities, Financial parameters and Optimisation target

Utilities	Use default financial parameters
Utility Prices	Plant lifetime (years) 20
Steam price (€/GJ)	Cost of capital (%) 8
4 	Yearly maintenance costs (% of TPC) (TPC: Total Process Costs) 2.5
Electricity price (€/MWh)	Yearly insurance costs (% of TPC)
	Yearly overhead and administrative costs (% of TPC) 0.3
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	@realise-ccus www.realiseccus.eu 14

Implementation of the optimisation target



Demonstration of the tool – Results

5 stacks, non-integrated results 5 stacks, integrated results (stack 1+2+3) ⊕ ⊝ 🭳 🖑 🏚 🚍 ⊕⊖ 🔍 🖑 🏚 🗏 40.0 60.0 • 50.0 **CO**2) 30.0 (ĩ) ton (€/ton 40.0 ē 30.0 20.0 of CO2 đ cost 20.0 Total 10.0 10.0 0.0 0.0 0.0 62.5 125.0 187.5 250.0 312.6 375.1 437.6 500.1 562.6 625.1 0.0 75.0 150.0 525.1 600.1 675.1 750.1 225.0 300.1 375.1 450.1 Yearly CO₂ capture rate (kton/yr) Yearly CO2 capture rate (kton/yr) ● Stacks CSF1 ● Stacks CSF2 ● Stacks CSF3 ● Stacks CSF4 ● Stacks CSF5 Stacks CSF123 Stacks CSF4 Stacks CSF5

Demonstration of the tool – results of the non-integrated case

Flue gas specific results								
Flow ID 个	CO₂ 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		
2	31715.84	6.35	17	33.76	5.03	4.18		
3	47573.77	7.77	17	33.76	7.54	4.76		
4	63431.69	8.98	17	33.76	10.05	5.21		
5	79289.61	10.04	17	33.76	12.57	5.6		

				0\	/erall resul	ts				
Flow ID	Total CO₂ captured (kton/yr)	Total CAPEX (M€)	Electricity demand (MWe)	Total heat demand (MW _{th})	Cooling water demand (MW _{th})	Solvent costs (€/ton CO₂)	Specific CAPEX (€/ton CO₂)	Specific variable OPEX (€/ton CO₂)	Specific fixed OPEX (€/ton CO₂)	Total costs (€/ton CO₂)
CSF1	125.02	22.95	1.17	15.9	16.93	4.86	18.7	23.38	10.66	52.73
CSF2	250.05	33.05	2.34	31.79	33.87	4.86	13.46	23.37	6.86	43.7
CSF3	375.07	41.81	3.51	47.69	50.8	4.86	11.35	23.37	5.46	40.19
CSF4	500.1	49.88	4.68	63.58	67.73	4.86	10.16	23.37	4.71	38.24
CSF5	625.12	57.5	5.86	79.48	84.66	4.86	9.37	23.37	4.23	36.97

Information can be quickly gathered on:

- Amount of CO₂ captured
- Major equipment sizing and costing
- Total utility demand (heat, electricity, cooling)
- Total CAPEX and OPEX calculations



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Practical information about the tool

The OCTOPUS tool is a free tool

An account can be requested by sending an email to me: jasper.ros@tno.nl

The tool can be accessed here: https://octopus.sensorlab.tno.nl/

An video introduction to the tool can be found here: <u>https://www.youtube.com/watch?v=mG8e6nQWP_8</u>

The tool contains an user manual to describe the structure of the tool and assumptions used for the calculations

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

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.



Future prospect of the tool

We are currently looking for opportunities to extend the tool, for example:

- Include other solvents (e.g. CESAR1)
- Include more detailed (cost) calculations on the integrated capture systems
- Include options for the user to constrain the tool (e.g. energy availability, plot space limitations)
- Include more capture rates (e.g. 99%)

Please contact us if you see possibilities to collaborate!



OCTOPUS Acknowledgements

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Thank you for listening



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